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# 1 First observation of $^{28}\text{O}$

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**Subjecting a physical system to extreme conditions is one of the means often employed to obtain a better understanding and deeper insight into its organization and structure. In the case of the atomic nucleus, one such approach is to investigate isotopes that have very different neutron-to-proton ( $N/Z$ ) ratios than in stable nuclei. Light neutron-rich isotopes exhibit the most asymmetric  $N/Z$  ratios and those lying beyond the limits of binding, which undergo spontaneous neutron emission and exist only as very short-lived resonances ( $\sim 10^{-21}$  seconds), provide the most stringent tests of modern nuclear structure theories. Here we report on the **first observation** of  $^{28}\text{O}$  and  $^{27}\text{O}$  via their decay into  $^{24}\text{O}$  and four and three neutrons. The  $^{28}\text{O}$  nucleus is of particular interest as, with 8 protons and 20 neutrons, it is expected in the standard shell model picture of nuclear structure to be one of a relatively small number of so-called “doubly-magic” nuclei. Both  $^{27}\text{O}$  and  $^{28}\text{O}$  were found to exist as narrow low-lying resonances and their decay energies are compared here to the results of sophisticated theoretical modelling, including a large-scale shell model calculation and a newly developed statistical approach. In both cases, the underlying nuclear interactions were derived from effective field theories of quantum chromodynamics. Finally, it is shown that the cross section for the production of  $^{28}\text{O}$  from a  $^{29}\text{F}$  beam is consistent with it not exhibiting a closed  $N = 20$  shell structure.**

32 One of the most active areas of present day nuclear physics  
33 is the investigation of rare isotopes with large  $N/Z$  imbal-  
34 ances. The structure of such nuclei provides for strong tests  
35 of our theories, including most recently, sophisticated *ab initio*  
36 type approaches whereby the underlying interactions between  
37 the constituent nucleons are constructed from first principles  
38 approaches (see, for example, ref.<sup>1</sup>).

39 Owing to the strong nuclear force, nuclei remain bound to  
40 the addition of many more neutrons than protons and the most  
41 extremely  $N/Z$  asymmetries are found for light neutron-rich  
42 nuclei (Fig. 1a). Here, beyond the limits of nuclear binding  
43 — the so-called neutron dripline — nuclei can exist as very  
44 short-lived ( $\sim 10^{-21}$  seconds) resonances, which decay by  
45 spontaneous neutron emission, with their energies and life-  
46 times dependent on the underlying structure of the system.  
47 Experimentally, such nuclei can only be reached for the light-  
48 est systems (Fig. 1a), where the location of the neutron dripline

49 has been established up to neon ( $Z = 10$ )<sup>2</sup> and the heaviest  
50 neutron unbound nucleus observed for fluorine ( $Z = 9$ )  $^{28}\text{F}$   
51 (ref.<sup>3</sup>). **Arguably the most extreme system, if confirmed to**  
52 **exist as a resonance, would be the tetra-neutron for which, a**  
53 **narrow near threshold continuum structure has been found in**  
54 **a recent missing mass measurement<sup>4</sup>.** Here we report on the  
55 direct observation of  $^{28}\text{O}$  ( $N/Z = 2.5$ ), which is unbound to 4  
56 neutron decay, and of neighbouring  $^{27}\text{O}$  (3 neutron unbound).

57 The nucleus  $^{28}\text{O}$  has long been of interest<sup>5,6</sup> as, in the stan-  
58 dard shell-model picture of nuclear structure, it is expected to  
59 be “doubly magic”. **Indeed, it** is very well established that  
60 for stable and near stable nuclei the proton and neutron num-  
61 bers 2, 8, 20, 28, 50, 82, 126 correspond to spherical closed  
62 shells<sup>7,8</sup>. Such nuclei represent a cornerstone in our under-  
63 standing of the structure of the many-body nuclear system. In  
64 particular, as considerable energy is required to excite them  
65 owing to the large shell gaps, they can be considered, when

66 modelling nuclei in their mass region, as an “inert” core with  
67 no internal degrees of freedom. Such an approach has his-  
68 torically enabled more tractable calculations to be made than  
69 attempting to model an  $A$ -body ( $A = Z + N$ ) nucleus from the  
70 full ensemble of nucleons. Indeed, this approach has been a  
71 fundamental premise of the shell model methods which have  
72 enabled an extremely wide variety of structural properties of  
73 nuclei to be described with good accuracy over a number of  
74 decades (see e.g., ref.<sup>9</sup>).

75 Of the very limited number of nuclei that are expected to  
76 be doubly magic based on the classical shell closures,  $^{28}\text{O}$  is,  
77 given its extreme  $N/Z$  asymmetry, the only one that is in prin-  
78 ciple experimentally accessible that has yet to be observed. In  
79 recent years, the doubly magic character of the two other such  
80 neutron-rich nuclei,  $^{78}\text{Ni}$  ( $Z = 28, N = 50; N/Z = 1.8$ )<sup>10</sup> and  
81  $^{132}\text{Sn}$  ( $Z = 50, N = 82; N/Z = 1.6$ )<sup>11</sup>, has been confirmed.  
82 The remaining candidate, two-neutron unbound nucleus  $^{10}\text{He}$   
83 ( $Z = 2, N = 8; N/Z = 4$ ), has been observed as a well-  
84 defined resonance but its magicity or otherwise has yet to be  
85 established (ref.<sup>12</sup>).

86 The  $N = 20$  shell closure has long been known, however,  
87 to disappear in the neutron-rich Ne, Na and Mg ( $Z = 10$ –  
88 12) isotopes (see, for example, refs.<sup>13,14</sup>). This region is re-  
89 ferred to as the “Island of Inversion” (IoI)<sup>15</sup>, whereby the en-  
90 ergy gap between the neutron  $sd$ - and  $pf$ -shell orbitals, rather  
91 than being well pronounced (Fig. 1b), is weakened or even  
92 vanishes and configurations with neutrons excited into the  
93  $pf$ -shell orbitals dominate the ground state (gs) of these nu-  
94 clei as shown schematically in Fig. 1c. The IoI nuclei with  
95 such configurations are well deformed, rather than spheri-  
96 cal, and exhibit low-lying excited states. Very recently, the  
97 IoI has been shown to extend to the fluorine isotopes  $^{28,29}\text{F}$   
98 ( $N = 19, 20$ )<sup>3,16–18</sup> which neighbour  $^{28}\text{O}$ . On the other hand,  
99 the last particle-bound oxygen isotope,  $^{24}\text{O}$  has been found to  
100 be doubly magic, with a new closed shell forming at  $N = 16$   
101 (refs.<sup>19–23</sup>). As such, the structural character of the more  
102 neutron-rich oxygen isotopes and, in particular,  $^{28}\text{O}$  is an in-  
103 triguing question. To date, however, only  $^{25,26}\text{O}$  ( $N = 17, 18$ )  
104 have been observed, as single- and two-neutron unbound sys-  
105 tems respectively<sup>24–27</sup>, with the latter existing as an extremely  
106 narrow, barely unbound resonance.

107 The present investigation focussed on the search for  $^{27,28}\text{O}$ ,  
108 produced in high-energy reactions, through the direct detec-  
109 tion of their decay products –  $^{24}\text{O}$  and 3 or 4 neutrons. Critical  
110 to the success of this work was the capability of the RIKEN  
111 RIBF (RI Beam Factory) to produce intense neutron dripline  
112 beams coupled to a thick active liquid hydrogen target system  
113 and a high performance multi-neutron detection array.

## 114 Experiment

115 The neutron-unbound  $^{27,28}\text{O}$  were produced via proton in-  
116 duced nucleon knockout reactions from a 235 MeV per nu-  
117 cleon beam of  $^{29}\text{F}$ . As depicted in Extended Data Fig. 1 the  
118  $^{29}\text{F}$  ions were characterised and tracked onto a thick (151 mm)  
119 liquid hydrogen reaction target using plastic scintillators and  
120 multi-wire drift chambers (MWDCs). The hydrogen target  
121 was surrounded by a time projection chamber (MINOS<sup>28</sup>)  
122 which allowed for the determination of the reaction vertex.  
123 This combination provided for both the maximum possible  
124 luminosity together with the ability to maintain a good  $^{27,28}\text{O}$   
125 decay energy resolution.

126 The forward focussed beam velocity reaction products –

127 charged fragments and fast neutrons – were detected and their  
128 momenta determined, using the SAMURAI spectrometer<sup>29</sup>  
129 including the three large-area segmented plastic scintillator  
130 walls of the NeuLAND<sup>30</sup> and NEBULA arrays. An overall  
131 detection efficiency for the 3 and 4 neutron decay of around  
132 2 and 0.4% was achieved for decay energies of  $\sim 0.5$  MeV  
133 (Extended Data Fig. 1). The decay energies were recon-  
134 structed from the measured momenta using the invariant-mass  
135 technique with a resolution (FWHM) of around 0.2 MeV at  
136  $\sim 0.5$  MeV decay energy (see Methods).

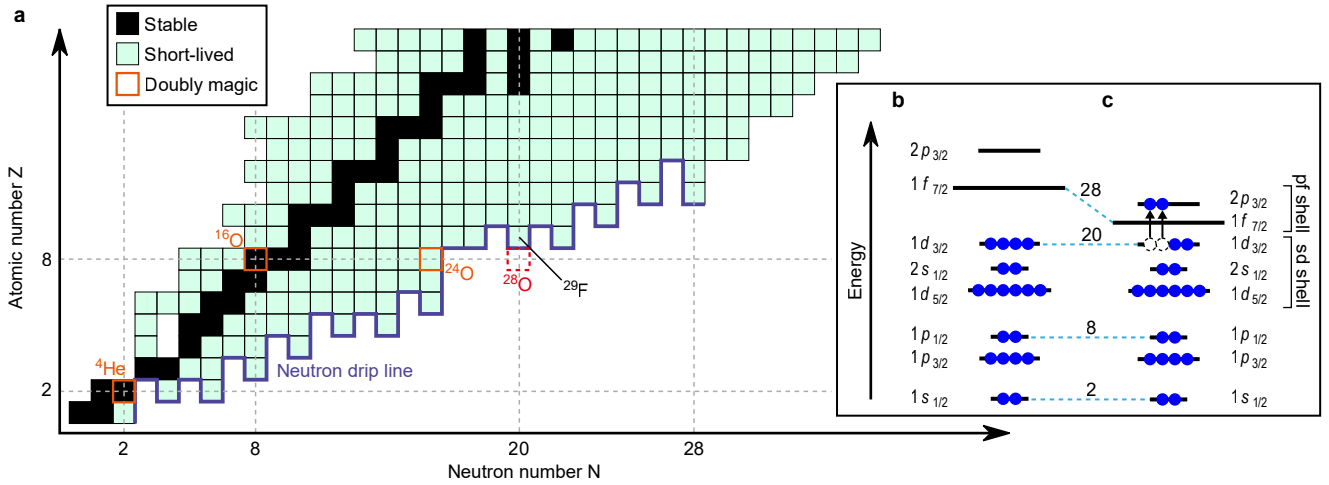
## 137 Analysis and results

138 The  $^{24}\text{O}$  fragments were identified by the magnetic rigid-  
139 ity, energy loss and time-of-flight derived from the SAMU-  
140 RAI spectrometer detectors. The neutrons incident on the  
141 NeuLAND and NEBULA arrays were identified based on the  
142 time-of-flight and energy deposited in the plastic scintillators.  
143 Importantly, the multi-neutron detection required the applica-  
144 tion of dedicated off-line analysis procedures in order to reject  
145 crosstalk (see Methods) – that is, events in which a neutron is  
146 scattered between and registered in two or more scintillators.

147 In the analysis, the decay neutrons were denoted  $n_1, n_2,$   
148  $\dots$  by ascending order of the two-body relative energy  $E_{0i}$   
149 between  $^{24}\text{O}$  and  $n_i$  – such that  $E_{01} < E_{02} < E_{03} < E_{04}$   
150 (Fig. 2d). The  $^{28}\text{O}$  decay energy,  $E_{01234}$ , reconstructed from  
151 the measured momentum vectors of the five decay particles,  
152 is shown in Fig. 2a. A narrow peak is clearly observed at  
153  $\sim 0.5$  MeV and may be assigned to be the  $^{28}\text{O}$  ground state.  
154 As a small fraction of crosstalk events could not be elimi-  
155 nated by the rejection procedures care must be taken to under-  
156 stand their contribution to the  $E_{01234}$  spectrum. In particular,  
157  $^{24}\text{O}+3n$  events, in which one of the neutrons creates crosstalk  
158 and is not identified as such in the analysis can mimic true  
159  $^{28}\text{O}$  decay. In this context, in order to provide a complete and  
160 consistent description of all the  $^{24}\text{O}+xn$  decay energy spec-  
161 tra, a full Monte-Carlo simulation was constructed (see Meth-  
162 ods). As shown in Fig. 2a the contribution from the residual  
163 cross talk events is found to be rather limited in magnitude in  
164 the  $^{24}\text{O}+4n$  decay energy spectrum and, moreover, produces  
165 a very broad distribution .

166 The decay of  $^{28}\text{O}$  was investigated by examining the corre-  
167 lations in the  $^{24}\text{O}$  plus neutrons subsystems (see Methods). In  
168 particular, the three-body ( $^{24}\text{O}+n_1+n_2$ ) partial decay energy  
169  $E_{012}$  (Extended Data Fig. 2a) was reconstructed from the  $^{24}\text{O}$   
170 +  $4n$  data set. The corresponding spectrum exhibits a sharp  
171 threshold peak arising from  $^{26}\text{O}_{\text{gs}}$ , which is known to have  
172 a decay energy of only 18(5) keV<sup>27</sup>. This observation clearly  
173 indicates that  $^{28}\text{O}$  sequentially decays through  $^{26}\text{O}_{\text{gs}}$  as shown  
174 by the arrows A and B in Fig. 2e.

175 We have also observed, in the  $^{24}\text{O}+3n$  channel, a  $^{27}\text{O}$  reso-  
176 nance for the first time, as may be seen in the four-body decay  
177 energy ( $E_{0123}$ ) spectrum of Fig. 2b. As confirmed by the simu-  
178 lations, which are able to simultaneously describe the  $^{24}\text{O}+3n$   
179 and  $4n$  decay energy spectra, the well populated peak-like  
180 structure below  $\sim 0.5$  MeV corresponds to  $^{28}\text{O}$  events where  
181 only three of the four emitted neutrons are detected. The  
182 peak at  $E_{0123} \sim 1$  MeV, however, cannot be generated by such  
183 events and must arise from a  $^{27}\text{O}$  resonance. This was con-  
184 firmed by the analysis of the data acquired with a  $^{29}\text{Ne}$  beam  
185 (see Methods and Extended Data Fig. 2e) where  $^{27}\text{O}$  can be  
186 produced by two-proton removal but not  $^{28}\text{O}$  as this requires  
187 the addition of a neutron. The  $^{27}\text{O}$  resonance also decays se-



**Fig. 1 | Nuclear chart and shell structure.** **a)** Nuclear chart up to  $Z = 18$  showing the stable and short-lived ( $\beta$ -decaying) nuclei. The experimentally established neutron dripline is shown by the thick blue line. Known doubly-magic nuclei are also indicated. **b)** Schematic illustration of the neutron configuration for a nucleus with a closed  $N = 20$  shell. **c)** The neutron configuration involving particle-hole excitations across a quenched  $N = 20$  shell gap.

188 sequentially via  $^{26}\text{O}_{\text{gs}}$  as shown by the arrows B and C in Fig. 2e  
 189 from the analysis of the partial decay energies (Extended Data  
 190 Figs.2c and d).

191 The decay energies of the  $^{27,28}\text{O}$  resonances were derived  
 192 from a fit of the  $E_{0123}$  spectrum with the condition that the par-  
 193 tial decay energy satisfies  $E_{012} < 0.08$  MeV (Fig. 2c) – that  
 194 is, decay via the  $^{26}\text{O}$  ground-state was selected so as to mini-  
 195 mize the uncertainties due to contributions from higher lying  
 196  $^{28}\text{O}$  resonances which were not identified in the present mea-  
 197 surements owing to the limited detection efficiency (Extended  
 198 Data Fig. 1). The fitting employed lineshapes which incor-  
 199 porated the effects of the experimental response functions, as  
 200 derived from the simulations, including the contribution aris-  
 201 ing from the residual crosstalk (see Methods).

202 In the case of  $^{28}\text{O}$  a decay energy of  
 203  $E_{01234} = 0.46^{+0.05}_{-0.04}(\text{stat}) \pm 0.02(\text{syst})$  MeV was found with  
 204 an upper limit of the width of the resonance of 0.7 MeV (68%  
 205 confidence interval). The cross section for single-proton  
 206 removal from  $^{29}\text{F}$  populating the resonance was deduced to be  
 207  $1.36^{+0.16}_{-0.14}(\text{stat}) \pm 0.13(\text{syst})$  mb. The systematic uncertainties  
 208 for the decay energy and the width were dominated by the  
 209 precise conditions employed in the neutron crosstalk rejection  
 210 procedures, while the principal contribution to that for the  
 211 cross section arose from the uncertainty in the neutron detec-  
 212 tion efficiency. It may be noted that if the resonance observed  
 213 here is an excited state of  $^{28}\text{O}$  (presumably the  $2^+$  level), then  
 214 the ground state must lie even closer to threshold and the  
 215 excitation energy of the former must be less than 0.46 MeV.  
 216 This, however, is very much lower than theory suggests  
 217 (2 MeV or more), even when the  $N = 20$  shell-closure is  
 218 absent (see below). As such, it is concluded that the ground  
 219 state has been observed.

220 In the case of  $^{27}\text{O}$  a decay energy of  
 221  $E_{0123} = 1.09 \pm 0.04(\text{stat}) \pm 0.02(\text{syst})$  MeV was found. The  
 222 width of the resonance was comparable to the estimated  
 223 experimental resolution of 0.22 MeV (FWHM). Nevertheless,  
 224 it was possible to obtain an upper limit on the width –  
 225 0.18 MeV (68% confidence interval) – through a fit of a  
 226 gated  $E_{012}$  spectrum for the much higher statistics  $^{24}\text{O}$  and

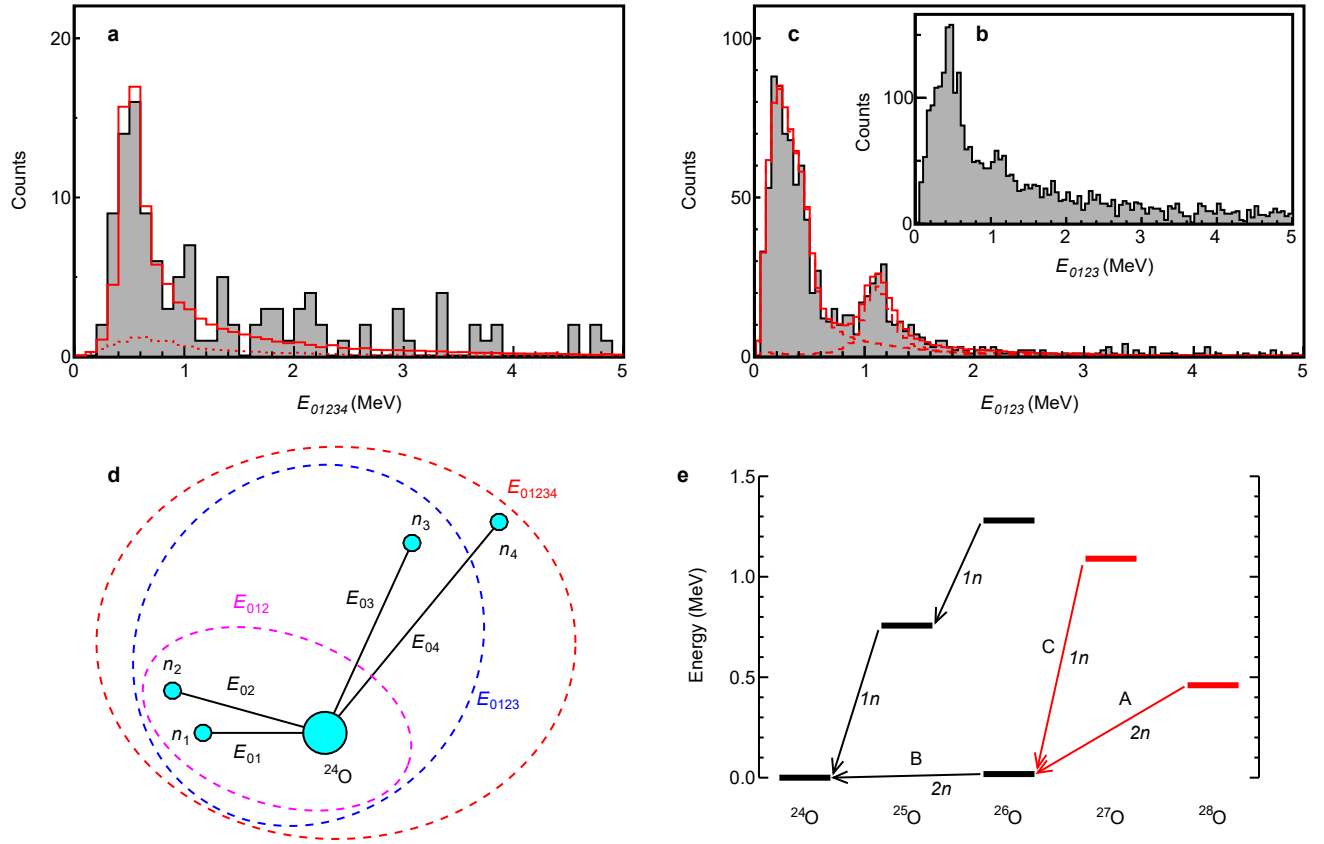
227 two-neutron coincidence events, as shown in Extended Data  
 228 Fig. 2f. The spin and parity ( $J^\pi$ ) of the resonance may be  
 229 tentatively assigned to be  $3/2^+$  or  $7/2^-$  based on the upper  
 230 limit of the width (see Methods).

### 231 Comparison to theory

232 The experimental ground-state energies of the oxygen iso-  
 233 topes  $^{25-28}\text{O}$  are summarized in Fig. 3 and compared to  
 234 theoretical calculations based on chiral effective field theory  
 235 ( $\chi$ EFT)<sup>32,33,37–40</sup> and large-scale shell model calculations<sup>9,34</sup>  
 236 including those with continuum effects<sup>35,36</sup>. We focus  
 237 on large-scale shell-model and coupled-cluster calculations,  
 238 where the latter is augmented with a novel statistical method.  
 239 Both techniques include explicitly three-nucleon forces which  
 240 are known to play a key role in describing the structure of  
 241 neutron-rich nuclei, including the oxygen isotopes and the lo-  
 242 cation of the  $Z = 8$  neutron dripline at  $^{24}\text{O}$  (refs.<sup>41–43</sup>).

243 The large-scale shell model calculations were undertaken  
 244 using the new EEdf3 interaction which was constructed based  
 245 on  $\chi$ EFT (see Methods). Since the calculations employ a  
 246 model space which includes the  $pf$  shell orbitals, the dis-  
 247 appearance of the  $N = 20$  shell closure can be naturally  
 248 described. The EEdf3 interaction is a modified version of  
 249 EEdf1<sup>32,33</sup>, which predicts correctly the neutron dripline at F,  
 250 Ne and Na, as well as a relatively low-lying  $^{29}\text{F}$  excited state<sup>17</sup>  
 251 and the appreciable occupancy of the neutron  $2p_{3/2}$  orbital<sup>3,18</sup>.  
 252 The EEdf3 interaction, which includes the effects of the EFT  
 253 three-nucleon forces<sup>44</sup>, provides a reasonable description of  
 254 the trends in the masses of the oxygen isotopes. However, as  
 255 may be seen in Fig. 3 it predicts somewhat higher  $^{27,28}\text{O}$  ener-  
 256 gies ( $\sim 1$  MeV) than found in the experiment. The calculated  
 257 sum of the occupation numbers for the neutron  $pf$ -shell or-  
 258 bitals is 2.5 (1.4) for  $^{28}\text{O}$  ( $^{27}\text{O}$ ) and for the  $1d_{3/2}$  orbital 2.0  
 259 (2.1), which are consistent with a collapse of the  $N = 20$  shell  
 260 closure. The EEdf3 calculations show that  $^{28}\text{O}_{\text{gs}}$  has large  
 261 admixtures of configurations involving neutron excitations in  
 262 the  $pf$ -shell orbitals as expected for nuclei in the IoI. This is  
 263 supported by the measured cross section as discussed below.

264 First-principle calculations were performed using the



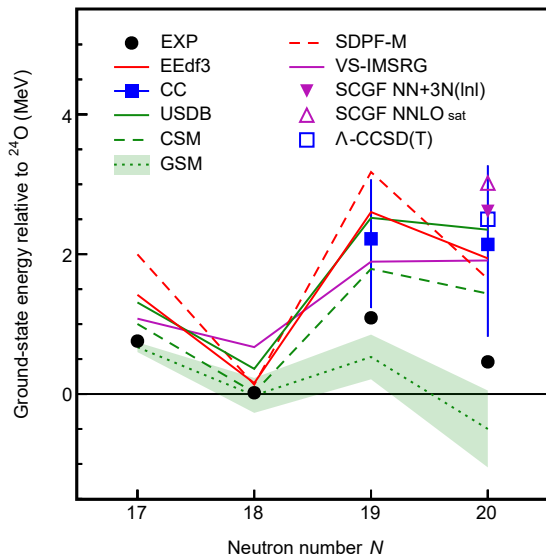
**Fig. 2 | Decay energy spectra and decay scheme.** **a)** Five-body decay energy ( $E_{01234}$ ) spectrum for  $^{24}\text{O}+4n$  events. The red-solid histogram shows the best-fit result taking into account the experimental response function. The dotted histogram shows the contribution arising from residual crosstalk that survives the rejection procedures (see Methods). **b)** Four-body decay energy ( $E_{0123}$ ) spectrum for  $^{24}\text{O}+3n$  events. **c)** Same as b, but gated by the partial decay energy  $E_{012} < 0.08$  MeV. The red-dashed histograms represent the contributions from  $^{28}\text{O}$  and  $^{27}\text{O}$  events, and the red-solid histogram shows the sum. **d)** Definition of the partial decay energies. **e)** Decay scheme of the unbound oxygen isotopes. The newly observed resonances and their decays are shown in red.

265 coupled-cluster (CC) method guided by history matching  
 266 (HM)<sup>45–47</sup> to explore the parameter space of the 17 low-  
 267 energy constants (LECs) in the  $\chi$ EFT description of the two-  
 268 and three-nucleon interactions. HM identifies the region of  
 269 parameter space for which the emulated CC method generates  
 270 non-implausible results (see Methods). A reliable low-  
 271 statistic sample of 121 different LEC parameterizations was  
 272 extracted for which the CC posterior predictive distribution  
 273 (ppd) was computed for the ground-state energies of  $^{27,28}\text{O}$ ,  
 274 which are shown in Fig. 3. The predicted  $^{27,28}\text{O}$  energies are  
 275 correlated, as is clearly seen in the plot of energy distributions  
 276 displayed in Extended Data Fig. 3. From this, the median values  
 277 and 68% credible regions were obtained for the  $^{27}\text{O}$ – $^{28}\text{O}$   
 278 and  $^{28}\text{O}$ – $^{24}\text{O}$  energy differences:  $\Delta E(^{27,28}\text{O})=0.11_{-0.39}^{+0.05}$  MeV  
 279 and  $\Delta E(^{28,24}\text{O})=2.1_{+1.2}^{-1.3}$  MeV. The experimental values  
 280  $\Delta E(^{27,28}\text{O})=0.63\pm 0.06(\text{stat})\pm 0.03(\text{syst})$  MeV and  
 281  $\Delta E(^{28,24}\text{O})=0.46_{-0.04}^{+0.05}(\text{stat})\pm 0.02(\text{syst})$  MeV, located at the  
 282 edge of the 68% credible region, are consistent with the CC  
 283 ppd. However, it is far enough away from the maximum to  
 284 suggest that only a few finely-tuned chiral interactions may be  
 285 able to reproduce the  $^{27}\text{O}$  and  $^{28}\text{O}$  energies. In addition, the  
 286 obtained credible regions of the  $^{27,28}\text{O}$  energies with respect  
 287 to  $^{24}\text{O}$  are relatively large, demonstrating that the measured  
 288 decay energies of the extremely neutron-rich isotopes  $^{27,28}\text{O}$

289 are valuable anchors for theoretical approaches based on  
 290  $\chi$ EFT.

291 In Fig. 3 the predictions of a range of other models are dis-  
 292 played. The USDB<sup>9</sup> effective interaction (constructed within  
 293 the  $sd$  shell) provides for arguably the most reliable predic-  
 294 tions of the properties of  $sd$ -shell nuclei. The continuum shell  
 295 model (CSM)<sup>35</sup> and the Gamow shell model (GSM)<sup>36</sup> include  
 296 the effects of the continuum, which should be important for  
 297 dripline and unbound nuclei. The shell-model calculation em-  
 298 ploying the SDPF-M interaction<sup>34</sup> includes the  $pf$  shell or-  
 299 bitals in its model space, which should be important if either  
 300 or both  $^{27,28}\text{O}$  lie within the IoI. All the calculations, except  
 301 those with the SDPF-M interaction, predict a  $J^\pi = 3/2^+ ^{27}\text{O}_{\text{gs}}$ .  
 302 In the case of the SDPF-M, a  $3/2^-$  ground state is found with  
 303 essentially degenerate  $3/2^+$  (energy plotted in Fig. 3) and  $7/2^-$   
 304 excited states at 0.71 MeV.

305 The remaining theoretical predictions are based on  $\chi$ EFT  
 306 interactions. The valence-space in-medium similarity renor-  
 307 malization group (VS-IMSRG)<sup>37</sup> employs the 1.8/2.0 (EM)  
 308 EFT potential<sup>44</sup>. The results for the self-consistent Green’s  
 309 function (SCGF) approach are shown for the NNLO<sub>sat</sub><sup>48</sup> and  
 310 NN+3N(InI) potentials<sup>38</sup>. The coupled-cluster calculation ( $\Lambda$ -  
 311 CCSD(T)<sup>39</sup>) using NNLO<sub>sat</sub> is also shown. Except for the re-  
 312 sults obtained using the GSM, all of the calculations shown  
 313 predict higher energies than found here for  $^{27}\text{O}$  and  $^{28}\text{O}$ .



**Fig. 3 | Ground-state energies with respect to  $^{24}\text{O}$ .** Experiment is shown by the filled circles where the values for  $^{27,28}\text{O}$  are the present results and those for  $^{25,26}\text{O}$  are taken from the atomic mass evaluation<sup>31</sup>. The experimental uncertainties are smaller than the symbol size. Comparison is made with predictions of shell-model calculations employing the EEdf3<sup>32,33</sup>, USDB<sup>9</sup> and SDPF-M<sup>34</sup> (see text for  $^{27}\text{O}$ ) interactions, the coupled-cluster method with the statistical approach (CC) and shell-model calculations incorporating continuum effects (CSM<sup>35</sup> and GSM<sup>36</sup>). Also shown are the predictions of *ab initio* approaches (VS-IMSRG<sup>37</sup>, SCGF<sup>38</sup>, and  $\Lambda$ -CCSD(T)<sup>39</sup>). The vertical bars for CC denote 68% credible intervals. The shaded band for GSM shows the uncertainties owing to *pf*-continuum couplings.

We now turn to the question of whether the  $N = 20$  shell closure occurs in  $^{28}\text{O}$ . Specifically, the measured cross section for single-proton removal from  $^{29}\text{F}$  may be used to deduce the corresponding spectroscopic factor ( $C^2S$ ) – a measure of the degree of overlap between initial and final state wave functions. As noted in the Introduction, the  $N = 20$  shell closure disappears in  $^{29}\text{F}$  and the ground state is dominated by neutron *pf*-shell configurations<sup>3,16–18</sup>. As such, if the neutron configuration of  $^{28}\text{O}$  is very similar to  $^{29}\text{F}$  and the  $Z = 8$  shell closure is rigid, the spectroscopic factor for proton removal will be close to unity. The spectroscopic factor was deduced using the distorted-wave impulse approximation (DWIA) approach (see Methods). As recent theoretical calculations predict  $J^\pi = 5/2^+$  or  $1/2^+$  for  $^{29}\text{F}_{\text{gs}}$  (see, for example, refs.<sup>3,32,33,49–51</sup>), the momentum distribution has been investigated (Extended Data Fig. 4) and was found to be consistent with proton removal from the  $1d_{5/2}$  orbital (see Methods), leading to a  $5/2^+$  assignment. The ratio of the measured to theoretical single-particle cross section provides for an experimentally deduced spectroscopic factor of  $C^2S = 0.48^{+0.05}_{-0.06}(\text{stat}) \pm 0.05(\text{syst})$ . Such an appreciable strength indicates that the  $^{28}\text{O}$  neutron configuration resembles quite strongly that of  $^{29}\text{F}$ . This value may be compared to that of 0.68 derived from the EEdf3 shell model calculations (where the center-of-mass correction factor<sup>52</sup>  $(29/28)^2$  has been applied). The 30% difference between the experimental  $C^2S$  as compared to theory, is in line with the well-known

reduction factor observed in (*p*, *2p*) and (*e*, *e'p*) reactions<sup>53</sup>. Importantly, the EEdf3 calculations predict admixtures of the ground state wave function of  $^{29}\text{F}$  with *sd*-closed-shell configurations of only some 12%. Consequently, even when the neutrons in  $^{28}\text{O}$  are confined to the *sd* shell a spectroscopic factor of only 0.13 is obtained. As such, it is concluded that, as in  $^{29}\text{F}$ , the *pf*-shell neutron configurations play a major role in  $^{28}\text{O}$  and that the  $N = 20$  shell closure disappears. Consequently the IoI extends to  $^{28}\text{O}$  and it is not a doubly-magic nucleus.

More effort will be required to properly quantify the character of the structure of  $^{28}\text{O}$  and the neutron *pf*-shell configurations. In this context, the determination of excitation energy of the first  $2^+$  state is the next step which may be envisaged experimentally<sup>17</sup>. The EEdf3 calculations predict an excitation energy of 2.097 MeV, which is close to that of  $\sim 2.5$  MeV computed by the particle rotor model assuming moderate deformation<sup>54</sup>. Both predictions are much lower than the energies found in doubly-magic nuclei – e.g., 6.917 MeV in  $^{16}\text{O}$  and 4.7 MeV in  $^{24}\text{O}$  (refs.<sup>21,23</sup>). A complementary probe of the neutron *sd* – *pf*-shell gap, which is within experimental reach, is the energy difference between the positive- and negative-parity states of  $^{27}\text{O}$  as seen in  $^{28}\text{F}$  (ref.<sup>3</sup>).

## Conclusions

We have reported here on the first observation of the extremely neutron-rich oxygen isotopes  $^{27,28}\text{O}$ . Both nuclei were found to exist as relatively low-lying resonances. These observations were made possible using a state-of-the-art setup which permitted the direct detection of 3 and 4 neutrons. From an experimental point of view, the multi-neutron-decay spectroscopy demonstrated here opens up new perspectives in the investigation of other extremely neutron-rich systems lying beyond the neutron dripline and the study of multi-neutron correlations. Comparison of the measured energies of  $^{27,28}\text{O}$  with respect to  $^{24}\text{O}$  with a broad range of theoretical predictions, including two approaches employing nuclear interactions derived from effective field theories of quantum chromodynamics, showed that in almost all cases theory underbinds both systems. The statistical coupled-cluster calculations indicated that the energies of  $^{27,28}\text{O}$  can provide valuable constraints of such *ab initio* approaches and, in particular, the interactions employed. Finally, while  $^{28}\text{O}$  is expected in the standard shell-model picture to be a doubly-magic nucleus ( $Z = 8$  and  $N = 20$ ), the single-proton removal cross section measured here, when compared to theory, was found to be consistent with it not having a closed neutron shell character. This result suggests that the island of inversion extends beyond  $^{28,29}\text{F}$  into the oxygen isotopes.

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## 532 METHODS

533 **Production of the  $^{29}\text{F}$  beam** The beam of  $^{29}\text{F}$  ions was pro-  
 534 vided by the RI Beam Factory operated by the RIKEN Nishina  
 535 Center and the Center for Nuclear Study (CNS), University  
 536 of Tokyo. It was produced by projectile fragmentation of an  
 537 intense 345 MeV per nucleon  $^{48}\text{Ca}$  beam on a 15-mm-thick  
 538 beryllium target. The secondary beam, including  $^{29}\text{F}$ , was pre-  
 539 pared using the BigRIPS<sup>55</sup> fragment separator operated with  
 540 aluminum degraders of 15-mm and 7-mm median thicknesses  
 541 at the first and fifth intermediate focal planes, respectively.  
 542 The primary  $^{48}\text{Ca}$  beam intensity was typically  $3 \times 10^{12}$  parti-  
 543 cles per second. The average intensity of the  $^{29}\text{F}$  beam was  
 544 90 particles per second.

545 **Measurement with a  $^{29}\text{Ne}$  beam** Data was also acquired to  
 546 measure the direct population of  $^{27}\text{O}$  via two-proton removal  
 547 from  $^{29}\text{Ne}$ . The beam was produced in a similar manner to  
 548 that for  $^{29}\text{F}$  and the energy was 228 MeV per nucleon with an  
 549 average intensity of  $8 \times 10^3$  particles per second.

550 Unfortunately, in this measurement the cross section for the  
 551 two-proton removal was much lower than expected and the  
 552 statistics obtained for  $^{24}\text{O}+3n$  coincidence events was too low  
 553 to be usefully exploited. Nevertheless, the decay of  $^{27}\text{O}$  could  
 554 be identified from the  $^{24}\text{O}+2n$  coincidence data. As may be  
 555 seen in **Extended Data Fig. 2e**, the three-body decay energy  
 556 ( $E_{012}$ ) spectrum gated by  $E_{01} < 0.08$  MeV – corresponding  
 557 to selection of the  $^{26}\text{O}$  ground-state decay – exhibits a clear  
 558 peak at around 1 MeV. As the simulations demonstrate, this  
 559 is consistent with the sequential decay of the  $^{27}\text{O}$  resonance  
 560 observed in the  $^{29}\text{F}$  beam data (Fig. 2c).

561 **Invariant-mass method** The invariant mass of  $^{28}\text{O}$ ,  
 562  $M(^{28}\text{O})$ , was reconstructed from the momentum vectors  
 563 of all the decay particles ( $^{24}\text{O}$  and  $4n$ ) with  $M(^{28}\text{O}) =$   
 564  $\sqrt{(\sum E_i)^2 - (\sum \mathbf{p}_i)^2}$ , where  $E_i$  and  $\mathbf{p}_i$  denote the total energy  
 565 and momentum vector of the decay particles. The decay en-  
 566 ergy is then obtained as  $E_{01234} = M(^{28}\text{O}) - M(^{24}\text{O}) - 4M_n$ ,  
 567 where  $M(^{24}\text{O})$  and  $M_n$  are the masses of  $^{24}\text{O}$  and the neu-  
 568 tron, respectively. The decay energy resolution is estimated by  
 569 Monte-Carlo simulations. The resolution (FWHM) varies as a  
 570 function of the decay energy approximately as  $0.14(E_{01234} +$   
 571  $0.87)^{0.81}$  MeV.

572 **Simulations** The experimental response functions, for both  
 573 the full and partial decay energy spectra, were derived from a  
 574 Monte-Carlo simulation based on GEANT4 (ref.<sup>56</sup>). All rele-  
 575 vant characteristics of the setup (geometrical acceptances and  
 576 detector resolutions) were incorporated, as well as those of  
 577 the beam, target and reaction effects. The QGSP\_INCLXX  
 578 physics class was adopted to describe the interactions of the  
 579 neutrons in the detectors (as well as non active material) as it  
 580 reproduces well the experimentally determined single-neutron  
 581 detection efficiency as well as the detailed characteristics of  
 582 neutron crosstalk events<sup>57,58</sup>. **The generated events treated us-**  
 583 **ing the same analysis procedure as for the experimental data.**  
 584 The overall efficiency as a function of decay energy for detect-  
 585 ing  $^{24}\text{O}$  and 3 and 4 neutrons, as estimated by the simulations,  
 586 is shown by the insets of Extended Data Fig. 1.

587 **Fitting of decay energy spectra** The energies, widths,  
 588 and amplitudes of the resonances, as modelled by intrinsic  
 589 lineshapes with a Breit-Wigner form with energy-dependent  
 590 widths, were obtained via fits of the corresponding decay en-  
 591 ergy spectra using the maximum likelihood method, where the  
 592 experimental responses were obtained by the simulations. As  
 593 the decays of both  $^{27}\text{O}$  and  $^{28}\text{O}$  proceed via the  $^{26}\text{O}$  ground

594 state (18 keV<sup>27</sup>), the width of which is very small, the ob-  
 595 served widths will be dominated by the one- and two-neutron  
 596 decay, respectively, to  $^{26}\text{O}$ . We assume an  $E_{01234}^2$  dependence  
 597 of the width for the  $2n$  emission<sup>59</sup> to  $^{26}\text{O}$  in the case of  $^{28}\text{O}$   
 598 and an energy dependence for the width of the single-neutron  
 599 emission<sup>60</sup> from  $^{27}\text{O}$  to  $^{26}\text{O}$ . Fits with orbital angular momen-  
 600 tum ( $L$ ) dependent widths ( $L = 2$  and 3) for the latter gave  
 601 consistent results within the statistical uncertainties.

602 A non-resonant component is not included in the fitting as  
 603 it is small, if not negligible, as in the cases of  $^{25,26}\text{O}$  produced  
 604 in one-proton removal reactions in previous experiments<sup>24–27</sup>.  
 605 The event selection with  $E_{012} < 0.08$  MeV should further  
 606 reduce any such contribution. As a quantitative check, a fit  
 607 with a non-resonant component — modelled with a lineshape  
 608 given by  $p_0 \sqrt{E_{0123}} \exp(-p_1 E_{0123})$ , where  $p_0$  and  $p_1$  are fitting  
 609 parameters — has been examined. This gives 8% reduction in  
 610 the  $^{28}\text{O}$  cross section with a very limited impact on the ener-  
 611 gies and widths of the  $^{27,28}\text{O}$  resonances.

612 **Neutron crosstalk** A single beam velocity neutron may  
 613 scatter between individual plastic scintillator detectors of the  
 614 three neutron walls of the setup. Such crosstalk events can  
 615 mimic true multi-neutron events and present a source of back-  
 616 ground. By examining the apparent kinematics of such events  
 617 and applying so-called causality conditions, this background  
 618 can be almost completely eliminated<sup>57,58</sup>. Importantly, both  
 619 the rejection techniques and the rate and characteristics of  
 620 the crosstalk have been benchmarked in and compared to the  
 621 simulations for dedicated measurements with single-neutron  
 622 beams.

623 In the case of the 4 neutron detection to identify  $^{28}\text{O}$  only  
 624 some 16% of the events arise from crosstalk which could not  
 625 be eliminated (Fig. 2a). The vast majority of these resid-  
 626 ual crosstalk events arise in cases when one (or occasionally  
 627 more) of the neutrons emitted in the decay of  $^{28}\text{O}$  is subject  
 628 to crosstalk. A very much smaller fraction is also estimated to  
 629 be produced when one of the three neutrons from the decay of  
 630  $^{27}\text{O}$ , produced directly by proton and neutron knockout, un-  
 631 dergoes crosstalk. Importantly the crosstalk cannot generate  
 632 a narrow peak-like structure in the  $E_{01234}$  decay energy spec-  
 633 trum.

634 **Partial decay energy of subsystems** The partial decay en-  
 635 ergies of the  $^{24}\text{O}+xn$  subsystems can be used to investigate  
 636 the manner in which  $^{27,28}\text{O}$  decay. In this analysis the de-  
 637 cay neutrons are numbered ( $n_1, n_2, \dots$ ) by ascending order  
 638 of two-body relative energy  $E_{0i}$  between  $^{24}\text{O}$  and  $n_i$  – that  
 639 is, such that,  $E_{01} < E_{02} < E_{03} < E_{04}$ . Of particular inter-  
 640 est here is the extremely low decay energy of the  $^{26}\text{O}$  ground  
 641 state (18 keV<sup>27</sup>), such that it appears just above zero energy  
 642 (or neutron-decay threshold) in the two-body partial decay en-  
 643 ergy  $E_{01}$  and three-body partial decay energy ( $E_{012}$ ).

644 Extended Data Figs. 2a and b display the distributions of  
 645 the partial decay energies  $E_{012}$  and  $E_{034}$  for the  $^{24}\text{O}+4n$  co-  
 646 incidence events with a total decay energy  $E_{01234} < 1$  MeV.  
 647 The resulting sharp threshold peak in the  $E_{012}$  spectrum is a  
 648 clear sign of sequential decay through the  $^{26}\text{O}$  ground state.  
 649 This is confirmed quantitatively by a simulation assuming  
 650 two-neutron emission to the the  $^{26}\text{O}$  ground state, which in  
 651 turn decays by two-neutron emission to the  $^{24}\text{O}$  ground state,  
 652 which describes well the  $E_{012}$  and  $E_{034}$  spectra. By compari-  
 653 son, a simulation assuming five-body phase space decay fails  
 654 to reproduce both of these spectra. We thus conclude that the  
 655  $^{28}\text{O}$  ground state sequentially decays via the  $^{26}\text{O}$  ground state



as depicted in Fig. 2e.

In a similar vein the sequential decay of  $^{27}\text{O}$  through the  $^{26}\text{O}$  ground state was identified from the analysis of the partial decay energies for the  $^{24}\text{O}+3n$  coincidence events. Extended Data Figs. 2c and d show the distributions of the partial decay energies  $E_{012}$  and  $E_{03}$  for events for which  $1.0 < E_{0123} < 1.2$  MeV. The  $E_{012}$  spectrum exhibits a strong enhancement at zero energy indicative of sequential decay through the  $^{26}\text{O}$  ground state. This interpretation is confirmed by the comparison shown with a simulation for the sequential decay of  $^{27}\text{O}$  including the contribution from the decay of  $^{28}\text{O}$ .

**Widths of the  $^{27,28}\text{O}$  resonances** As the energy of the  $^{28}\text{O}$  resonance is lower than those of  $^{27}\text{O}$  and  $^{25}\text{O}$  (Fig. 2e), both one- and three-neutron emission are energetically forbidden. The two-neutron decay to the  $^{26}\text{O}$  ground state and the four-neutron decay to  $^{24}\text{O}$  are allowed with nearly equal decay energies. The former decay should be favoured as the effective few-body centrifugal barrier increases according to the number of emitted particles<sup>59</sup>. It may be noted that the upper limit of 0.7 MeV observed here for the  $^{28}\text{O}$  resonance width is consistent with the theoretical estimates for its sequential decay<sup>59</sup>.

The upper limit for the  $^{27}\text{O}$  width (0.18 MeV) may be compared to the single-particle widths<sup>61</sup> for neutron decay. Since the width of  $^{26}\text{O}$  is very narrow due to the extremely small decay energy (18 keV<sup>27</sup>), the  $^{27}\text{O}$  width should be dominated by the one for the first step  $^{27}\text{O} \rightarrow ^{26}\text{O}+n$ . The widths for  $s$ ,  $p$ ,  $d$ ,  $f$ -wave neutron emission are 5, 3, 0.8, 0.06 MeV. Assuming that the corresponding spectroscopic factors are not small ( $\geq 0.1$ ), this would suggest that the decay occurs via  $d$ - or  $f$ -wave neutron emission. As such, the spin and parity of the  $^{27}\text{O}$  resonance may be tentatively assigned to be  $3/2^+$  or  $7/2^-$ .

**Momentum distribution** Extended Data Fig. 4 shows the transverse momentum ( $P_x$ ) distribution of the  $^{24}\text{O}+3n$  system in the rest frame of the  $^{29}\text{F}$  beam for events gated by  $E_{012} < 0.08$  MeV and  $E_{0123} < 0.8$  MeV – that is, events corresponding to population of the  $^{28}\text{O}$  ground state. We note that this analysis employed the  $^{24}\text{O}+3n$  events as the limited  $^{24}\text{O}+4n$  statistics could not be usefully exploited in distinguishing between the momentum distributions for the proton knockout from different orbitals. Even though the momentum distribution is slightly broadened by the undetected decay neutron, it still reflects directly the character of the knocked-out proton.

The experimental  $P_x$  distribution is compared to DWIA (Distorted Wave Impulse Approximation) reaction theory calculations (see below) for knockout of a proton from the  $1d_{5/2}$  and  $2s_{1/2}$  orbitals. The theoretical distributions are convoluted with the experimental resolution as well as the much smaller broadening induced by the undetected neutron ( $\sigma = 34$  MeV/c). The best fit normalization of the theoretical distribution obtained by the distorting potential with the Dirac phenomenology (microscopic folding model potential) through a  $\chi^2$  minimization gives reduced- $\chi^2$  values of 2.0 (2.0) for the  $1d_{5/2}$  proton knockout and 3.7 (4.7) for the  $2s_{1/2}$  knockout. The curves in Extended Data Fig. 4 represent the calculations obtained by the distorting potential with the Dirac phenomenology. The better agreement for the  $1d_{5/2}$  proton knockout suggests that the spin and parity of the  $^{29}\text{F}$  ground state is  $5/2^+$  as predicted by the shell model calculations, including those using the EEdf3 interaction.

**EEdf3 calculations** The EEdf3 Hamiltonian<sup>32</sup> is a variant of the EEdf1 Hamiltonian, which was used in ref.<sup>33</sup> for describing F, Ne, Na, and Mg isotopes up to neutron dripline<sup>32</sup>. The EEdf1 Hamiltonian was derived from chiral effective field theory ( $\chi$ EFT) interaction, as described below. The  $\chi$ EFT interaction proposed by Entem and Machleidt<sup>62,63</sup> was taken with  $\Lambda = 500$  MeV, as the nuclear force in vacuum, up to the next-to-next-to-next-to-leading-order ( $\text{N}^3\text{LO}$ ) in the  $\chi$ EFT. It was then renormalized using the  $V_{\text{low-}k}$  approach<sup>64,65</sup> with a cutoff of  $\Lambda_{V_{\text{low-}k}} = 2.0$  fm<sup>-1</sup>, in order to obtain a low-momentum interaction decoupled from high-momentum phenomena. The EKK method<sup>66–68</sup> was then adopted in order to obtain the effective NN interaction for the  $sd$ - $pf$  shells, by including the so-called  $\hat{Q}$ -box, which incorporates unfolded effects coming from outside of the model space<sup>69</sup>, up to third order and its folded diagrams. As to the single-particle basis vectors, the eigenfunctions of the three-dimensional harmonic oscillator potential were taken as usual. In addition, the contributions from the Fujita Miyazawa three-nucleon force (3NF)<sup>70</sup> were added in the form of the effective NN interaction<sup>41</sup>. The Fujita Miyazawa force represents the effects of the virtual excitation of a nucleon to a  $\Delta$  baryon by pion-exchange processes and includes the effects of  $\Delta$ -hole excitations, but does not include other effects such as contact ( $c_D$  and  $c_E$ ) terms.

In the present study, we explicitly treat neutrons only, while the protons remained confined to the  $^{16}\text{O}$  closed-shell core. As such, there is no proton-neutron interaction between active nucleons, and the neutron-neutron interaction is weaker. As this increases the relative importance of the effects from 3NF, we adopt the more modern 3NF of Hebeler et al.<sup>44</sup>, which is expected to have finer details and improved properties. We obtain effective NN interactions from this 3NF first by deriving density-dependent NN interactions from them<sup>71</sup> and then by having the density dependence integrated out with the normal density. It was suggested that this 3NF produces results similar to those reported in ref.<sup>33</sup> for the F, Ne, Na and Mg isotopes. As a result of this change, the single-particle energies are shifted for the  $1d_{5/2}$  and  $2s_{1/2}$  orbitals by  $-0.72$  MeV, for the  $1d_{3/2}$  orbital by  $-0.42$  MeV and for the  $pf$  shell orbitals by  $0.78$  MeV.

**Coupled-cluster calculations and emulators** The starting point for the calculations is the intrinsic Hamiltonian,

$$H = T_{\text{kin}} - T_{\text{CoM}} + V_{NN} + V_{NNN}. \quad (1)$$

Here  $T_{\text{kin}}$  is the kinetic energy,  $T_{\text{CoM}}$  the kinetic energy of the center-of-mass, and  $V_{NN} + V_{NNN}$  are nucleon-nucleon and three-nucleon potentials from  $\chi$ EFT<sup>62,72,73</sup> and include Delta isobars<sup>74</sup>. The momentum space cutoff of this interaction is  $\Lambda = 394$  MeV/c.

We used the coupled-cluster method<sup>75–81</sup> with singles-doubles and perturbative triples excitations, known as the CCSDT-3 approximation<sup>82,83</sup>, to compute the ground-state energy of  $^{28}\text{O}$ , and the particle-removed equation-of-motion (EOM) coupled-cluster method from refs.<sup>84,85</sup> for the ground-state energy of  $^{27}\text{O}$ . The coupled-cluster calculations start from a spherical Hartree-Fock reference of  $^{28}\text{O}$  in a model-space of 13 major harmonic oscillator shells with an oscillator frequency of  $\hbar\omega = 16$  MeV. The three-nucleon force is limited to three-body energies up to  $E_{3\text{max}} = 14\hbar\omega$ . For energy differences the effects of model-space truncations and coupling to the scattering continuum are small and were neglected in the

777 history matching analysis.

778 The low-energy constants (LECs) of this interaction are  
 779 constrained by a history matching approach employing high-  
 780 precision emulators enabled by eigenvector continuation<sup>86</sup>.  
 781 These tools mimic the results of actual coupled-cluster com-  
 782 putations, but are several orders of magnitude faster to eval-  
 783 uate, hence facilitating comprehensive exploration of the rel-  
 784 evant parameter space. The emulators work as follows. In  
 785 the 17-dimensional space of LECs, the parameterization of  
 786 the  $\Delta\text{NNLO}_{\text{GO}}(394)$  potential<sup>74</sup> serves as a starting point  
 787 around which we select emulator training points according to  
 788 a space-filling lattice hypercube design for which we perform  
 789 coupled-cluster computations of ground-state energies, radii,  
 790 and excited states of  $^{16,22,24}\text{O}$  (see Extended Data Table 1 for  
 791 details). Keeping track of the variations of the observables  
 792 and the corresponding coupled-cluster eigenstates as the low-  
 793 energy constants are varied, allows us to construct an emu-  
 794 lator that can be used to predict the results for novel param-  
 795 eterizations. This emulator strategy is rather general<sup>87</sup> and  
 796 possible because the eigenvector trajectory generated by con-  
 797 tinuous changes of the low-energy constants only explores a  
 798 relatively small subspace of Hilbert space. Eigenvector con-  
 799 tinuation emulation tailored to coupled-cluster eigenstates is  
 800 referred to as the subspace-projected coupled-cluster (SP-CC)  
 801 method. In this work, we extended the SP-CC method of  
 802 ref.<sup>88</sup> to excited states and increased the precision by includ-  
 803 ing triples excitations via the CCSDT-3 and EOM-CCSDT-3  
 804 methods, respectively. Our SP-CC emulators employ up to 68  
 805 training points for each observable of interest, and use model  
 806 spaces consisting of 11 major harmonic oscillator shells. We  
 807 checked the precision of each emulator by performing emula-  
 808 tor diagnostics<sup>89</sup>: confronting the emulator predictions with  
 809 the results of actual coupled-cluster computations, see Ex-  
 810 tended Data Fig. 5. Once constructed, the emulators are in-  
 811 expensive computational tools that can precisely predict the  
 812 results for virtually arbitrary parameterizations of the EFT po-  
 813 tentials. This allows us to explore several hundred million  
 814 parameterizations with the computational cost of only a few  
 815 hundred actual coupled-cluster computations. The use of emu-  
 816 lation hence represents a critical advance, that facilitates a far  
 817 deeper analysis of the coupled-cluster method, that was previ-  
 818 ously infeasible due to the substantial computational expense  
 819 of the coupled-cluster calculations. Hence, these techniques  
 820 overcome a major barrier to the use of such coupled-cluster  
 821 methods.

822 **Coupled-cluster calculations: Linking models to reality**  
 823 We describe the relationship between experimental observa-  
 824 tions,  $z$ , and *ab initio* model predictions  $M(\theta)$ , where  $\theta$  de-  
 825 notes the parameter vector of the theoretical model, as

$$z = M(\theta) + \epsilon_{\text{method}} + \epsilon_{\text{model}} + \epsilon_{\text{exp}}. \quad (2)$$

826 In this relation, we consider experimental uncertainties,  $\epsilon_{\text{exp}}$ ,  
 827 as well as method approximation errors  $\epsilon_{\text{method}}$ . The latter  
 828 represent, e.g., model-space truncations and other approxima-  
 829 tions in the *ab initio* many-body solvers and are estimated  
 830 from method convergence studies<sup>74</sup>. Most importantly, we  
 831 acknowledge the fact that even if we were to evaluate the  
 832 model  $M(\theta)$  at its best possible choice of the parameter vec-  
 833 tor,  $\theta^*$ , the model output,  $M(\theta^*)$ , would still not be in ex-  
 834 act quantitative agreement with reality due to, e.g., simplifi-  
 835 cations and approximations inherent to the model. We de-  
 836 scribe this difference in terms of a model discrepancy term,

837  $\epsilon_{\text{model}}$ . The expected EFT-convergence pattern of our model  
 838 allows us to specify further probabilistic attributes of  $\epsilon_{\text{model}}$   
 839 a priori<sup>90–93</sup>. We employ the model errors defined in<sup>94</sup>. The  
 840 use of emulators based on eigenvector continuation<sup>86–88</sup> pro-  
 841 vides us with an efficient approximation,  $\tilde{M}(\theta)$ , of the model.  
 842 This approach entails an emulator error  $\epsilon_{\text{emulator}}$  such that  
 843  $M(\theta) = \tilde{M}(\theta) + \epsilon_{\text{emulator}}$ , as outlined in the previous section.  
 844 Obviously, we do not know the exact values of the errors in  
 845 Eq. (2), hence we represent them as uncertain quantities and  
 846 specify reasonable forms for their statistical distributions, in  
 847 alignment with the Bayesian paradigm. This allows for these  
 848 uncertainties to be formally incorporated in all subsequent cal-  
 849 culations and inferences. We also assume that the errors add  
 850 independently of each other and the inputs  $\theta$ .

851 **Coupled-cluster calculations: History matching** In this  
 852 work we use an iterative approach for complex computer mod-  
 853 els known as history matching (HM)<sup>45–47</sup> in which the model,  
 854 solved at different fidelities, is confronted with experimental  
 855 data  $z$  using relation (2). The aim of HM is to estimate the  
 856 set  $\mathcal{Q}(z)$  of values for  $\theta$ , for which the evaluation of a model  
 857  $M(\theta)$  yields an acceptable—or at least not implausible (NI)—  
 858 match to a set of observations  $z$ . HM has been employed in  
 859 various studies<sup>95–97</sup> ranging, e.g., from effects of climate mod-  
 860 eling<sup>98,99</sup> to systems biology<sup>47</sup>. The present work represents  
 861 the first application in nuclear physics. We introduce the stan-  
 862 dard implausibility measure

$$I^2(\theta) = \max_{i \in \mathcal{Z}} \frac{|\tilde{M}_i(\theta) - z_i|^2}{\text{Var}(\tilde{M}_i(\theta) - z_i)}, \quad (3)$$

863 which is a function over the input parameter space and quan-  
 864 tifies the (mis-)match between our (emulated) model output  
 865  $\tilde{M}_i(\theta)$  and the observation  $z_i$  for all observables  $i$  in the tar-  
 866 get set  $\mathcal{Z}$ . This specific definition uses the maximum of the  
 867 individual implausibility measures (one for each observable)  
 868 as the restricting quantity. We consider a particular value for  
 869  $\theta$  as implausible if  $I(\theta) > c_I \equiv 3.0$  appealing to Pukelsheim’s  
 870 three-sigma rule<sup>100</sup>. In accordance with the assumptions lead-  
 871 ing to Eq. (2), the variance in the denominator of Eq. (3) is a  
 872 sum of independent squared errors. Generalizations of these  
 873 assumptions are straightforward if additional information on  
 874 error covariances or possible inaccuracies in our error model  
 875 would become available. An important strength of the HM  
 876 approach is that we can proceed iteratively, excluding regions  
 877 of input space by imposing cutoffs on implausibility measures  
 878 that can include *additional* observables  $z_i$  and corresponding  
 879 model outputs  $M_i$ , and possibly refined emulators  $\tilde{M}_i$ , as the  
 880 iterations proceed. The iterative HM proceeds in waves ac-  
 881 cording to a straightforward strategy that can be summarized  
 882 as follows:

- 883 1. At iteration  $j$ : Evaluate a set of model runs over the  
 884 current NI volume  $\mathcal{Q}_j$  using a space-filling design of  
 885 sample values for the parameter inputs  $\theta$ . Choose a re-  
 886 jection strategy based on implausibility measures for a  
 887 set  $\mathcal{Z}_j$  of informative observables.
- 888 2. Construct or refine emulators for the model predictions  
 889 across the current non-implausible volume  $\mathcal{Q}_j$ .
- 890 3. The implausibility measures are then calculated over  
 891  $\mathcal{Q}_j$ , using the emulators, and implausibility cutoffs are  
 892 imposed. This defines a new, smaller NI volume  $\mathcal{Q}_{j+1}$   
 893 which should satisfy  $\mathcal{Q}_{j+1} \subset \mathcal{Q}_j$ .

894 4. Unless (a) the emulator uncertainties for all observ-  
 895 ables of interest are sufficiently small in comparison to  
 896 the other sources of uncertainty, (b) computational re-  
 897 sources are exhausted, or (c) all considered points in  
 898 the parameter space are deemed implausible, we:

- 899 – include any additional informative observables in  
 900 the considered set  $\mathcal{Z}_{j+1}$ , and return to step 1.

901 5. If 4(a) or (b) is true we generate a large number of ac-  
 902 ceptable runs from the final NI volume  $\mathcal{Q}_{\text{final}}$ , sampled  
 903 according to scientific need.

904 The *ab initio* model for the observables we consider comprises  
 905 at most 17 parameters; 4 subleading pion-nucleon couplings,  
 906 11 nucleon-nucleon contact couplings, and 2 short-ranged  
 907 three-nucleon couplings. To identify a set of NI parameter  
 908 samples we performed iterative HM in four waves using ob-  
 909 servables and implausibility measures as summarized in Ex-  
 910 tended Data Table 1. For each wave we employ a sufficiently  
 911 dense latin hypercube set of several million candidate param-  
 912 eter samples. For the model evaluations we utilized fast com-  
 913 putations of neutron-proton (*np*) scattering phase shifts and  
 914 efficient emulators for the few- and many-body observables  
 915 listed. See Extended Data Table 2 for the list of included ob-  
 916 servables and key information for each wave. The input vol-  
 917 ume for wave 1 included large ranges for the relevant param-  
 918 eters, as indicated by the panel ranges in the lower left triangle  
 919 of Extended Data Fig. 6. In all four waves, the input volume  
 920 for  $c_{1,2,3,4}$  is a four-dimensional hypercube mapped onto the  
 921 multivariate Gaussian pdf resulting from a Roy-Steiner analy-  
 922 sis of  $\pi N$  scattering data<sup>101</sup>. In wave 1 and wave 2 we sampled  
 923 all relevant parameter directions for the set of included two-  
 924 nucleon observables. In wave 3, the additional  ${}^3\text{H}$  and  ${}^4\text{He}$   
 925 observables were added. Since they are known to be rather  
 926 insensitive to the four model parameters acting solely in the  
 927 *P*-wave, we therefore ignored this subset of the inputs and  
 928 compensated by slightly enlarging the corresponding method  
 929 errors. This is a well-known emulation procedure called in-  
 930 active parameter identification<sup>45</sup>. For the final iteration, i.e.  
 931 wave 4, we considered all 17 model parameters and added a  
 932 set of observables for the oxygen isotopes  ${}^{16,22,24}\text{O}$  and emu-  
 933 lated the model outputs for  $5 \times 10^8$  parameter samples. Ex-  
 934 tended Data Fig. 6 summarizes the sequential NI volume re-  
 935 duction, wave-by-wave, and indicates the set  $\mathcal{Q}_4$  of 634 NI  
 936 samples after the fourth and final wave. The volume reduc-  
 937 tion is guided by the implausibility measure (3) and the op-  
 938 tical depths (see Eqs. (25) and (26) in ref.<sup>47</sup>), where the lat-  
 939 ter are illustrated in the lower left triangle of Extended Data  
 940 Fig. 6. The NI samples summarise the parameter region of  
 941 interest, and can directly aid insight regarding interdependen-  
 942 cies between parameters induced by the match to observed  
 943 data. This region is also where we would expect the poste-  
 944 rior distribution to reside. We see that the iterative history  
 945 matching process trains a nested series of emulators that be-  
 946 come more and more accurate over this posterior region, as  
 947 the iterations progress.

948 **Coupled-cluster calculations: Bayesian posterior sam-**  
 949 **pling** The NI samples in the final HM wave also serve as  
 950 excellent starting points for extracting the posterior probabili-  
 951 ty density function (pdf) of the parameters  $\theta$ , i.e.  $p(\theta|A =$   
 952  $2 - 24)$ . To this end, we assume a normally distributed likeli-  
 953 hood, according to Eq. (2), and a uniform prior corresponding  
 954 to the initial volume of wave 1. Note that the prior for  $c_{1,2,3,4}$

955 is the multivariate Gaussian resulting from a Roy-Steiner anal-  
 956 ysis of  $\pi N$  scattering data<sup>101</sup>. We sample the posterior using  
 957 the affine invariant Markov Chain Monte Carlo ensemble sam-  
 958 pler emcee<sup>102</sup> and the resulting distribution is shown in the up-  
 959 per right triangle of Extended Data Fig. 6. The sampling was  
 960 performed with four independent ensemble chains, each with  
 961 150 walkers, and satisfactory convergence was reached (diag-  
 962 nosed using the Gelman-Rubin test with  $|\hat{R} - 1| < 10^{-4}$  in all  
 963 dimensions). We performed  $5 \cdot 10^5$  iterations per walker—after  
 964 an initial warm-up of 5000 steps—and kept one final sample  
 965 for every 500 steps. Combining all chains we therefore end up  
 966 with  $4 \times 150 \times 1000 = 6 \cdot 10^5$  final samples. In addition, we  
 967 explored the sensitivity of our results to modifications of the  
 968 likelihood definition. Specifically, we used a student-t distri-  
 969 bution ( $\nu = 5$ ) to see the effects of allowing heavier tails, and  
 970 we introduced an error covariance matrix to study the effect  
 971 of correlations ( $\rho \approx 0.6$ ) between selected observables. In the  
 972 end, the differences in the extracted credibility regions was not  
 973 great and we therefore present only results obtained with the  
 974 uncorrelated, multivariate normal distribution (see Extended  
 975 Data Table 3).

976 A subset of marginal posterior predictive distributions (ppd)  
 977 are shown in Extended Data Fig. 7. Clearly, a subset of 100  
 978 samples provides an accurate low-statistics representation of  
 979 this marginalized ppd. We exploit this feature in our final pre-  
 980 dictions for  ${}^{27,28}\text{O}$  presented in the main text. Note that the  
 981 ppd does not include draws from the model discrepancy pdf.  
 982 To include information about the  ${}^{25}\text{O}$  separation energy with  
 983 respect to  ${}^{24}\text{O}$  we perform a straightforward Bayesian update  
 984 of the posterior pdf  $p(\theta|A = 2 - 24)$  for the LECs. This com-  
 985 plements the statistical analysis of the *ab initio* model with  
 986 important information content from an odd and neutron-rich  
 987 oxygen isotope. Using the pdf  $p(\theta|A = 2 - 24)$  we draw  
 988 500 model predictions for  $\Delta E({}^{25,24}\text{O})$  and account for all in-  
 989 dependent and normally distributed uncertainties according to  
 990 Extended Data Table 1. Next, we draw 121 different LEC pa-  
 991 rameterizations from the updated posterior and use coupled  
 992 cluster to compute the corresponding ground-state energies of  
 993  ${}^{27,28}\text{O}$ . The full bivariate ppd for the  ${}^{28}\text{O}$ - ${}^{24}\text{O}$  and  ${}^{27}\text{O}$ - ${}^{28}\text{O}$   
 994 energy differences,  $\Delta E({}^{28,24}\text{O})$  and  $\Delta E({}^{27,28}\text{O})$ , with asso-  
 995 ciated credible regions, are shown in Extended Data Fig. 3.  
 996 The effect of the continuum on the energy difference was es-  
 997 timated to be  $\sim 0.5$  MeV in ref.<sup>39</sup> and was neglected in this  
 998 work. We note that our ability to examine the full ppd for these  
 999 expensive *ab initio* calculations provides welcome additional  
 1000 insight, which is a direct consequence of the use of the HM  
 1001 procedure. We note that a sufficiently precise determination  
 1002 of  $\Delta E({}^{28,24}\text{O})$  and  $\Delta E({}^{27,28}\text{O})$  requires wave 4 in the history  
 1003 matching and also using the separation energy  $\Delta E({}^{24,25}\text{O})$  for  
 1004 the construction of the pdf. Without input about  ${}^{25}\text{O}$ , the sep-  
 1005 aration energy  $\Delta E({}^{27,28}\text{O})$  becomes too uncertain to be use-  
 1006 ful. It is in this sense that a sufficiently precise prediction  
 1007 of  $\Delta E({}^{27,28}\text{O})$  is finely tuned and cannot be based only on  
 1008 the properties of light nuclei up to  ${}^4\text{He}$ . Changes in the low-  
 1009 energy constants that have small impact in few nucleon sys-  
 1010 tems are magnified in  ${}^{28}\text{O}$ . Apparently, one needs information  
 1011 about all nuclear shells including the *sd* shell to meaningfully  
 1012 predict this key nucleus.

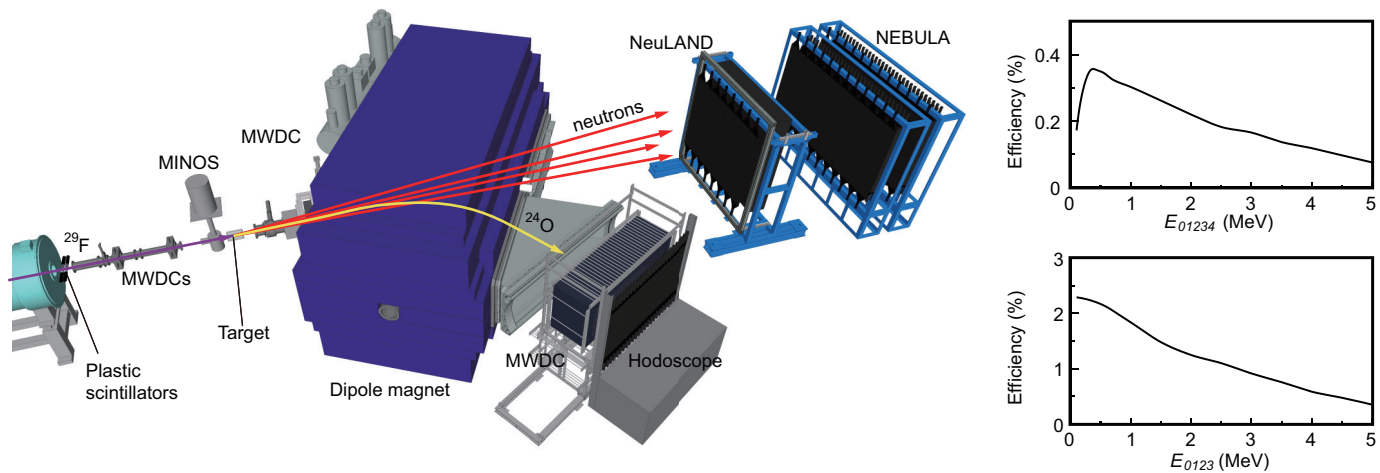
1013 **DWIA calculations** The distorted-wave impulse approx-  
 1014 imation (DWIA)<sup>53,103,104</sup> describes proton-induced proton  
 1015 knockout – (*p*, *2p*) – processes as proton-proton (*pp*) elas-  
 1016 tic scattering. This is referred to as the impulse approxima-

- tion, which is considered to be valid at intermediate energies when both outgoing protons have large momenta with respect to the residual nucleus. The DWIA approach has been successful in describing proton-induced knockout reactions; in ref.<sup>53</sup>, it was shown that the spectroscopic factors deduced from  $(p, 2p)$  reactions for the single-particle levels near the Fermi surface of several nuclei are consistent with those extracted from electron-induced  $(e, e'p)$  reactions. The transition matrix of  $(p, 2p)$  processes within DWIA theory is given by  $T_{p2p} = \langle \chi_1 \chi_2 | t_{pp} | \chi_0 \phi_p \rangle$ , where  $\chi_i$  are the distorted waves of the incoming proton (0) and the outgoing two protons (1 and 2), whereas  $\phi_p$  is the normalized bound-state wave function of the proton inside the nucleus. The  $pp$  effective interaction is denoted by  $t_{pp}$ , the absolute square of which is proportional to the  $pp$  elastic cross section. The nonlocality corrections<sup>105</sup> to both  $\chi_i$  and  $\phi_p$  are taken into account as well as the Moller factor<sup>106</sup> for  $t_{pp}$  that guarantees the Lorentz invariance of the  $pp$  reaction probability. The  $(p, 2p)$  cross section is given by  $F_{\text{kin}} C^2 S |T_{p2p}|^2$  with  $F_{\text{kin}}$  being a kinetic factor and  $C^2 S$  the spectroscopic factor.
- In this study, the cross section integrated over the allowed kinematics of the outgoing particles was calculated. We employed the Franey-Love parameterization<sup>107</sup> for  $t_{pp}$  and the Bohr-Mottelson's (BM) single-particle potential<sup>108</sup> in order to compute  $\phi_p$ . We have used two types of the one-body distorting potential to obtain  $\chi$  – specifically, the Dirac phenomenology (set EDAD2<sup>109</sup>) and a microscopic folding model potential based on the Melbourne  $G$ -matrix interaction<sup>110</sup> and one-body nuclear densities calculated with the BM single-particle model<sup>108</sup>. It was found that the difference in the  $(p, 2p)$  cross sections calculated with the two sets of distorting potentials was at most 7.5%. In addition, they give almost identical shapes for the momentum distributions. As such, we have adopted here the average value of the cross sections for each single-particle configuration.
- Data availability** Source data for Figs. 2a-c, Extended Data Figs. 2a-f, and Extended Data Fig. 4 are provided with this paper. All of the other relevant data that support the findings of this study are available from the corresponding author upon reasonable request.
- Code availability** Our unpublished computer codes used to generate the results reported in this paper are available from the corresponding author upon reasonable request.
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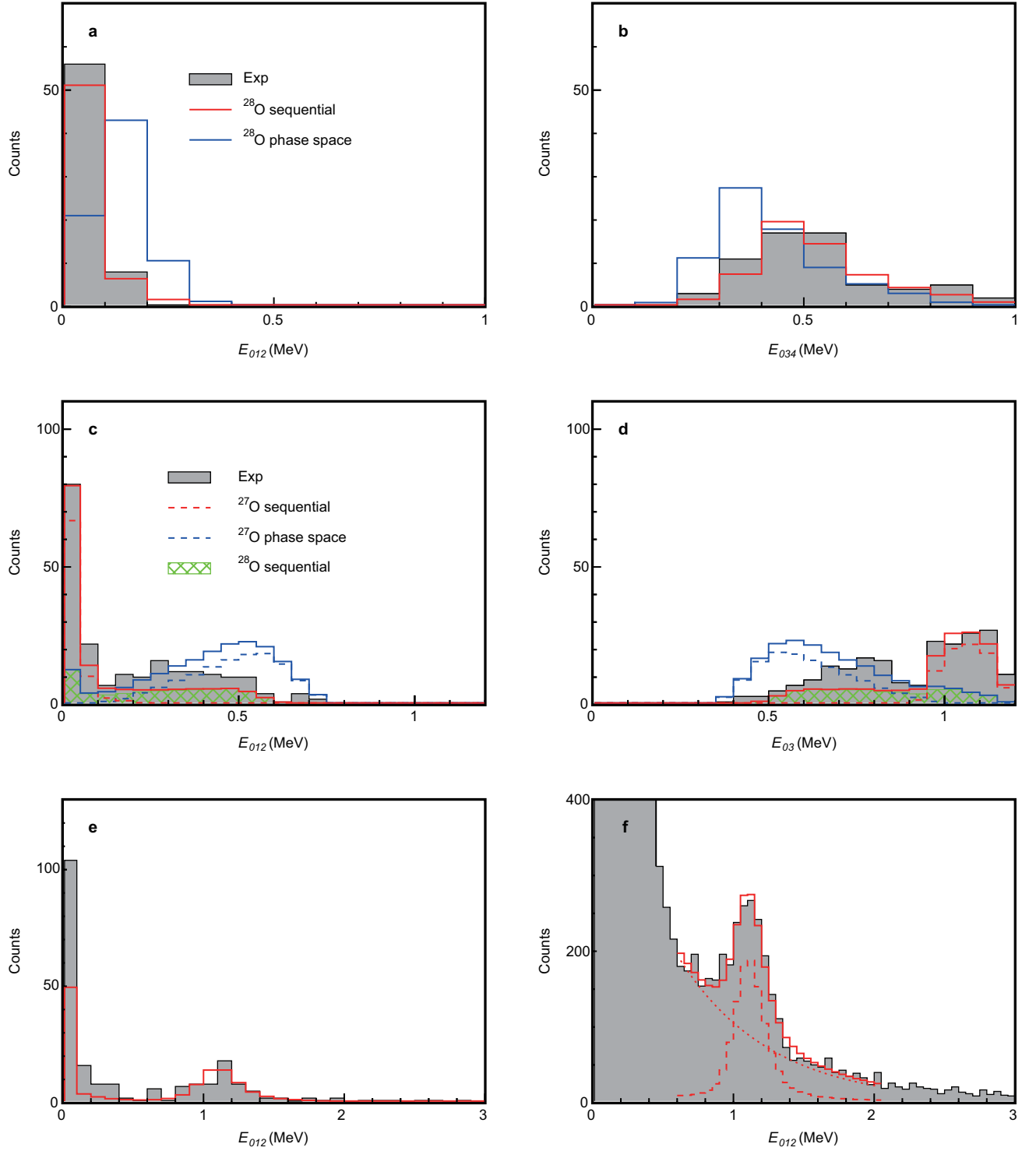
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- 1262 **Author Contributions** Y.K. designed and proposed the experiment, performed the offline analysis and the Monte Carlo simulations. Y.K., T.N., T.O., K.O., and N.A.O. drafted the manuscript. Y.K., T.N., N.L.A, H.F., L.A., T.A., H.B., K.B., C.C., D.C., H.C., N.C., A.C., F.D., A.D., Q.D., Z.D., C.A.D., Z.E., I.G., J.-M.G., J.G., A.G., M.N.H., A.H., C.R.H., M.H., A.H., Á.H., J.W.H., T.I., J.K., N.K.-N., S.K., S.K., K.K., T.K., D.K., S.K., I.K., V.L., S.L., F.M.M., S.M., J.M., K.M., T.M., M.N., K.N., N.N., T.N., A.O., F.O.S., N.A.O., H.O., T.O., V.P., S.P., A.R., D.R., A.T.S., T.S., M.S., H.S., Y.S., H.S., F.S., P.S., M.S., Y.S., H.S., D.S., O.S., L.S., S.T., M.T., M.T., H.T., Y.T., T.T., J.T., J.T., T.U., H.W., Z.Y., M.Y., and K.Y. took part in the setting up of the experiment and/or monitored the data accumulation and/or maintained the operation of experiment

1276 and detectors. T.O., N.S., N.T., Y.U. and S.Y. performed the  
1277 EEdf3 calculations. K.O. performed the DWIA calculations.  
1278 A.E., C.F., G.H., W.G.J., T.P., Z.H.S., and I.V. performed the  
1279 coupled-cluster calculations and their statistical analysis and  
1280 wrote the associated sections of the manuscript.

1281 **Competing Interests** The authors declare no competing in-  
1282 terests.

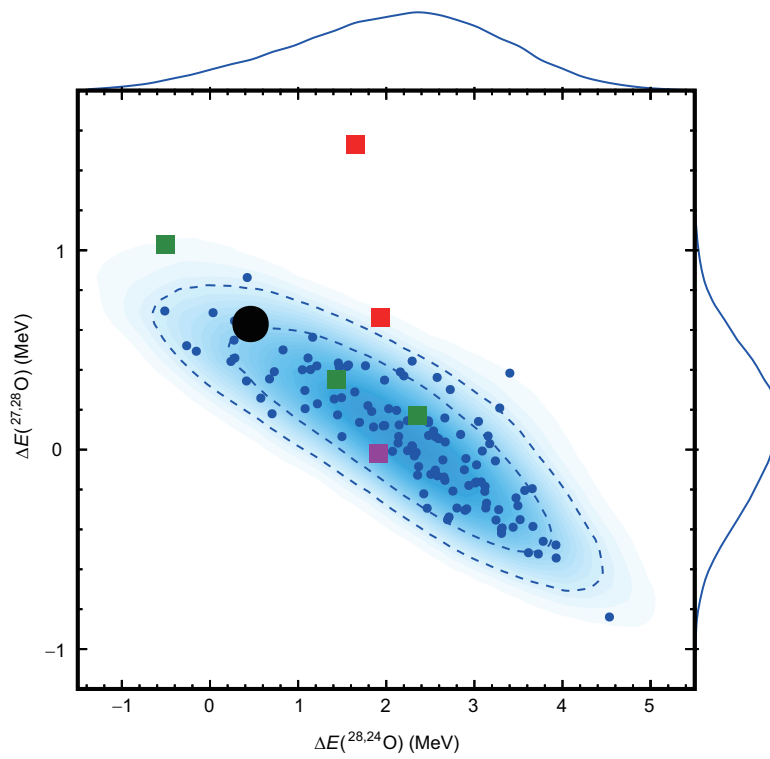


**Extended Data Fig. 1 | Schematic view of the experimental setup.** The insets show the overall efficiency as a function of decay energy for detecting  $^{24}\text{O} + 3$  and 4 neutrons.

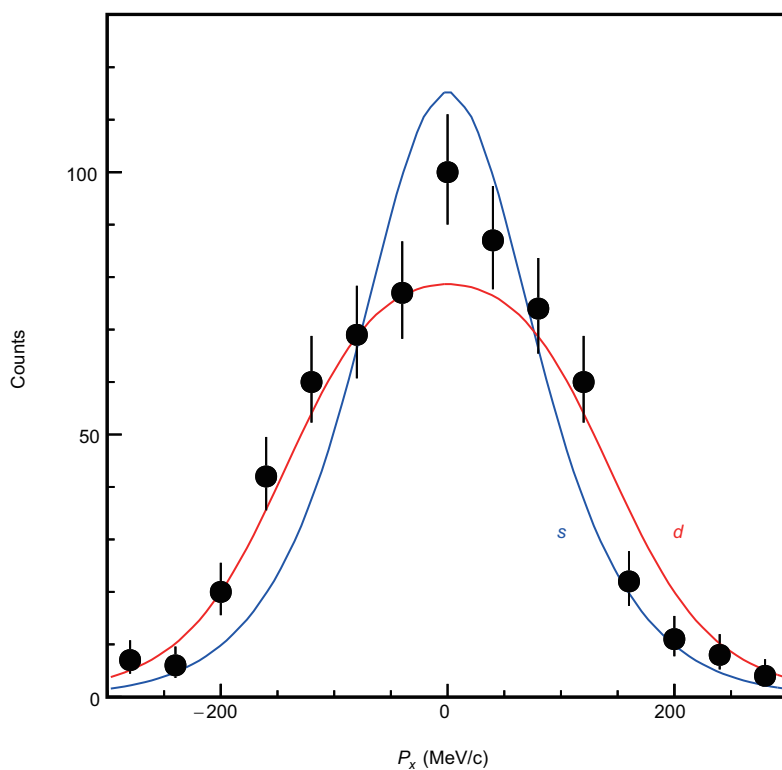


**Extended Data Fig. 2 | Partial decay energy spectra.** **a**, The filled grey histogram is the three-body decay energy  $E_{012}$  gated on the total decay energy  $E_{01234} < 1$  MeV for the  $^{24}\text{O}+4n$  coincidence events. The red and blue histograms are the results of simulations of sequential decay via the  $^{26}\text{O}$  ground state (A and B in Fig. 2e) and five-body phase space decay, respectively. **b**, Same as a, but for the three-body decay energy  $E_{034}$ . **c**, The filled grey histogram is the partial decay energy spectrum  $E_{012}$  gated by  $1.0 < E_{0123} < 1.2$  MeV for the  $^{24}\text{O}+3n$  coincidence events. The red and blue dashed histograms are the results of simulations assuming  $^{27}\text{O}$  sequential (B and C in Fig. 2e) and four-body phase space decay, respectively. The green hatched histogram represents the contribution from the decay of  $^{28}\text{O}$ . The red (blue) solid histogram is the sum of the contributions from  $^{28}\text{O}$  and  $^{27}\text{O}$  for sequential (phase space) decay. **d**, Same as c, but for the two-body decay energy  $E_{03}$ . **e**, Decay energy spectrum of  $^{24}\text{O}+2n$  events from the  $^{29}\text{Ne}$  beam data. The grey histogram represents events with  $E_{01} < 0.08$  MeV. The red histogram shows the results of the simulation for the decay of the  $^{27}\text{O}$  resonance. The excess observed near zero decay energy is interpreted as arising from direct population of the  $^{26}\text{O}$  ground state from  $^{29}\text{Ne}$ . **f**, Decay energy spectrum of  $^{24}\text{O}+2n$  events from the  $^{29}\text{F}$  beam. The grey histogram represents events with  $E_{01} < 0.08$  MeV. The red histogram shows the best fit in the region of the peak arising from the decay of the  $^{27}\text{O}$  resonance (dashed histogram) and an exponential distribution (dotted curve) arising from all other contributions which come primarily from the decay of  $^{28}\text{O}$ .

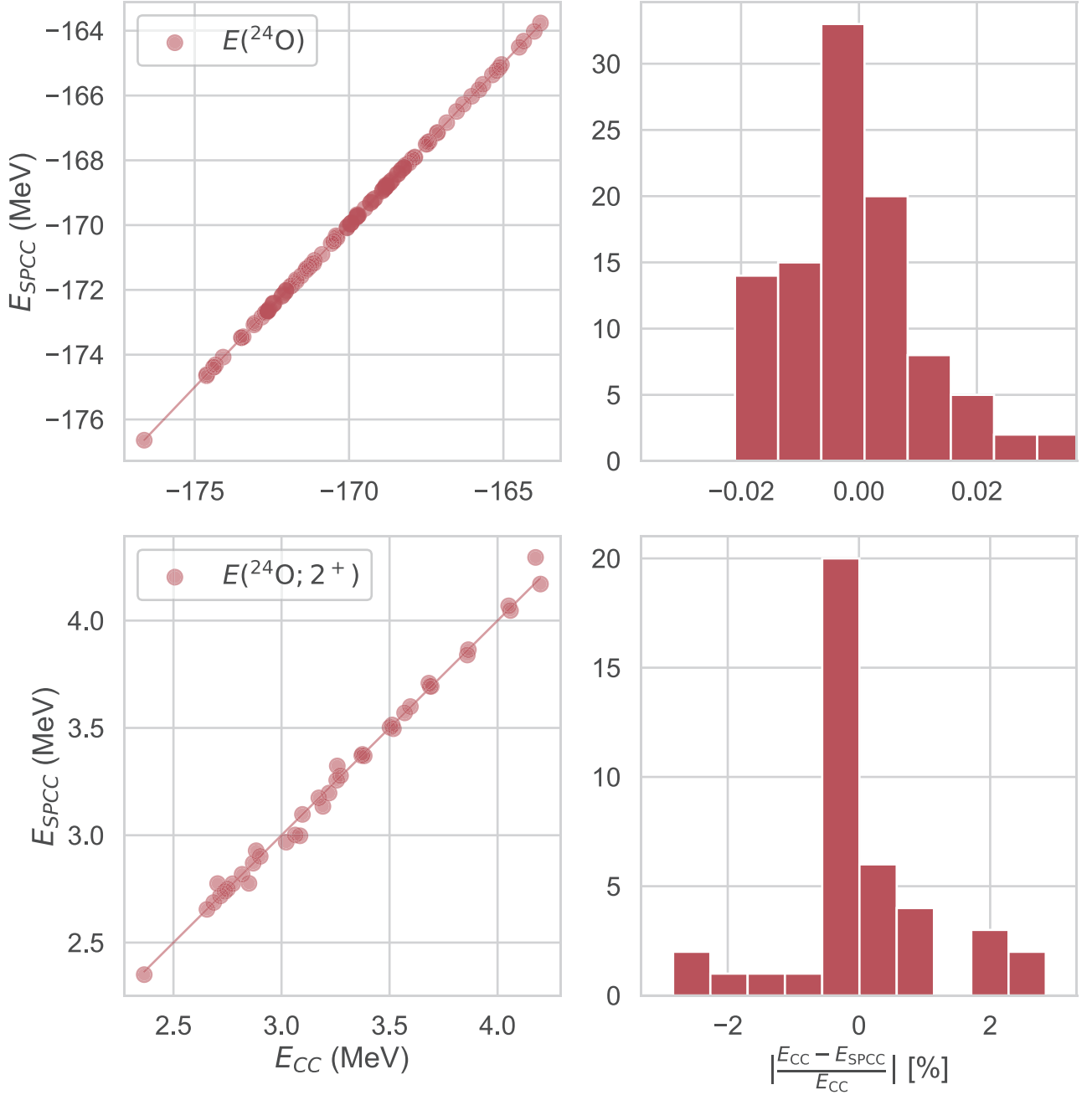




**Extended Data Fig. 3 | Probability distribution of the calculated energy differences.** Survived non-implausible calculations are shown by blue dots as functions of energy differences  $\Delta E(^{28,24}\text{O})$  and  $\Delta E(^{27,28}\text{O})$ . The black circle shows experiment. The dashed curves indicate 68% and 90% highest probability density regions. The top and right distributions are the 1-dimensional probability density distributions. The values given by the other theories are plotted as squares: green – USDB, GSM, and CSM, red –SDPF-M and EEdf3 and purple – VS-IMSRG.



**Extended Data Fig. 4 | Transverse momentum distribution of the  $^{24}\text{O}+3n$  system in the rest frame of the  $^{29}\text{F}$  beam.** Events corresponding to the population of the  $^{28}\text{O}$  ground state ( $E_{012} < 0.08$  MeV and  $E_{0123} < 0.8$  MeV) are shown by the data points. The blue and red solid lines represent the DWIA calculations, including the experimental effects for  $s_{1/2}$  and  $d_{5/2}$  proton knockout, respectively, whereby the distributions have been scaled to best fit experiment.

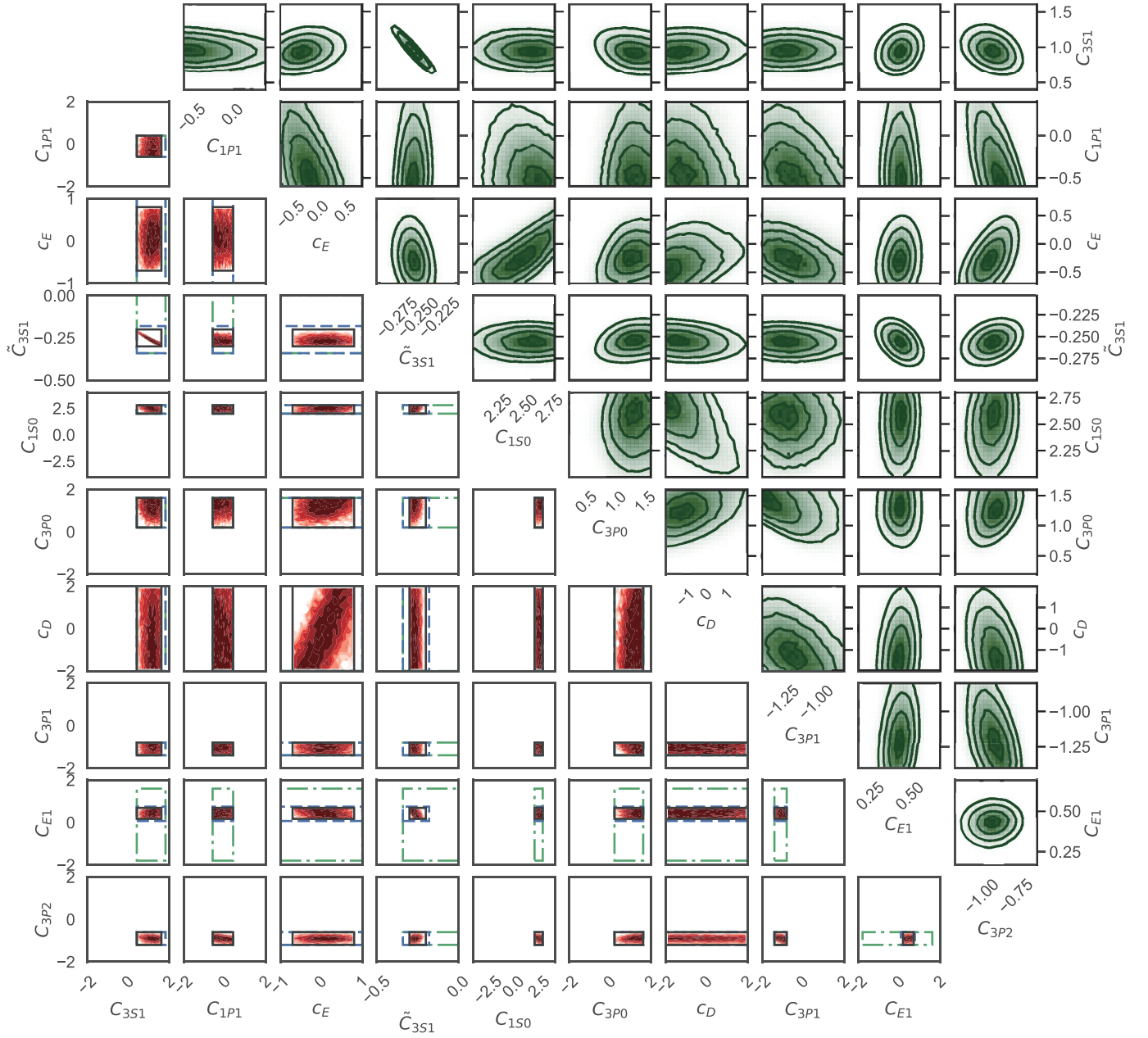


**Extended Data Fig. 5 | Cross-validation of emulators.** (Upper left panel) Total energies of  $^{24}\text{O}$  computed with the coupled-cluster method in the CCSDT-3 approximation versus the SP-CC emulator for a validation set of 100 parameter samples. (Upper right panel) Distribution of residuals in percent. (Lower left panel)  $2^+$  excitation energies of  $^{24}\text{O}$  computed with the coupled-cluster method in the EOM-CCSDT-3 approximation versus the SP-CC emulator for a validation set of 40 parameter samples. (Lower right panel) Distribution of residuals in percent.

Target	$z$	$\epsilon_{\text{exp}}$	$\epsilon_{\text{model}}$	$\epsilon_{\text{method}}$	$\epsilon_{\text{emulator}}$
$E(^2\text{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p^2(^2\text{H})$	3.9030	0.0	0.02	0.0005	0.001%
$Q(^2\text{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\text{H})$	-8.4818	0.0	0.17	0.0005	0.005%
$E(^4\text{He})$	-28.2956	0.0	0.55	0.0005	0.005%
$r_p^2(^4\text{He})$	2.1176	0.0	0.045	0.0005	0.05%
$E(^{16}\text{O})$	127.62	0.0	0.75	1.5	0.5%
$r_p^2(^{16}\text{O})$	6.660	0.0	0.16	0.05	1%
$\Delta E(^{22,16}\text{O})$	-34.41	0.0	0.4	0.5	1%
$\Delta E(^{24,22}\text{O})$	-6.35	0.0	0.4	0.5	4%
$E_{2^+}(^{24}\text{O})$	4.79	0.0	0.5	0.25	2%
$\Delta E(^{25,24}\text{O})$	0.77	0.02	0.4	0.25	—

**Extended Data Table 1 | Error assignments used in the statistical analysis.** Energies in (MeV), squared point-proton radii in ( $\text{fm}^2$ ) and the deuteron quadrupole moment in ( $e^2\text{fm}^2$ ).  $\Delta E(^{25,24}\text{O})$  is used in the Bayesian update step and the experimental target is from Hoffman et al.<sup>24</sup>. This observable is computed in particle-attached coupled-cluster theory<sup>84</sup> and does not involve an emulator.

Target	$z$	$\epsilon_{\text{exp}}$	$\epsilon_{\text{model}}$	$\epsilon_{\text{method}}$	$\epsilon_{\text{emulator}}$
$E(^2\text{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p^2(^2\text{H})$	3.9030	0.0	0.02	0.0005	0.001%
$Q(^2\text{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\text{H})$	-8.4818	0.0	0.17	0.0005	0.005%
$E(^4\text{He})$	-28.2956	0.0	0.55	0.0005	0.005%
$r_p^2(^4\text{He})$	2.1176	0.0	0.045	0.0005	0.05%
$E(^{16}\text{O})$	127.62	0.0	0.75	1.5	0.5%
$r_p^2(^{16}\text{O})$	6.660	0.0	0.16	0.05	1%
$\Delta E(^{22,16}\text{O})$	-34.41	0.0	0.4	0.5	1%
$\Delta E(^{24,22}\text{O})$	-6.35	0.0	0.4	0.5	4%
$E_{2^+}(^{24}\text{O})$	4.79	0.0	0.5	0.25	2%
$\Delta E(^{25,24}\text{O})$	0.77	0.02	0.4	0.25	—



**Extended Data Fig. 6 | History-matching waves and Bayesian posterior sampling.** (Lower left triangle) The panel limits correspond to the input volume of wave 1. The domain is iteratively reduced and the input volumes of wave 2, 3, 4 are indicated by green/dash-dotted, blue/dashed, black/solid rectangles. The optical depths of non-implausible samples in the final wave are shown in red with darker regions corresponding to a denser distribution of non-implausible samples. (Upper right triangle) Parameter posterior pdf from MCMC sampling with the non-implausible samples of the history-matching analysis as starting points. We use an uncorrelated, multivariate normal likelihood function and a uniform prior bounded by the first wave initial volume. Note that the relevant posterior regions are small in some directions, but larger in others such as  $c_D$  and  $c_E$ .

Wave	Target set ( $Z$ )	Number of active parameters	Number of input samples	NI samples fraction
1	$np$ phase shifts	5–7	$10^5$ – $10^7$	$10^{-1}$ – $10^{-4}$
2	$A = 2$	7	$10^8$	$2.3 \cdot 10^{-4}$
3	$A = 2$ –4	13	$10^8$	$3.4 \cdot 10^{-5}$
4	$A = 2$ –4, 16–24	17	$5 \cdot 10^8$	$1.3 \cdot 10^{-6}$

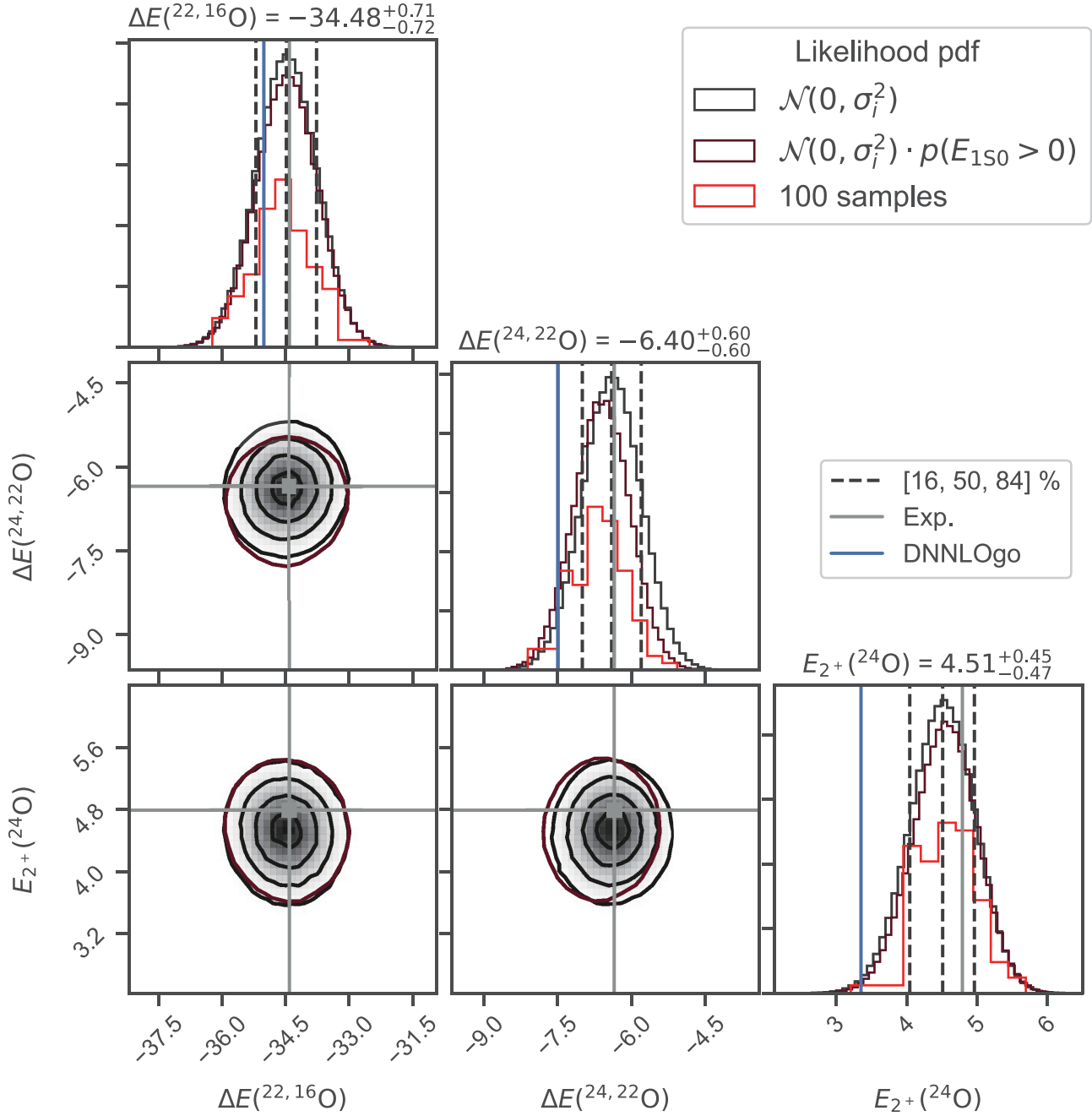
**Extended Data Table 2 | Definitions of history-matching waves used in this work.** The  $np$  phase shifts correspond to six targets ( $T_{\text{lab}} = 1, 5, 25, 50, 100, 200$  MeV) for  $^1S_0, ^3S_1, ^1P_1, ^3P_0, ^3P_1, ^3P_2$  partial waves. The  $A = 2$  observables are  $E(^2\text{H}), r_p(^2\text{H}), Q(^2\text{H})$ , while  $A = 3, 4$  are  $E(^3\text{H}), E(^4\text{He}), r_p(^4\text{He})$ . Finally,  $A = 16 - 24$  correspond to  $E(^{16}\text{O}), r_p(^{16}\text{O})$ , the binding-energy differences  $\Delta E(^{24,22}\text{O}), \Delta E(^{22,16}\text{O})$  and  $E_{2^+}(^{24}\text{O})$ .

Wave	Target set ( $Z$ )	Number of active parameters	Number of input samples	NI samples fraction
1	$np$ phase shifts	5–7	$10^5$ – $10^7$	$10^{-1}$ – $10^{-4}$
2	$A = 2$	7	$10^8$	$2.3 \cdot 10^{-4}$
3	$A = 2$ –4	13	$10^8$	$3.4 \cdot 10^{-5}$
4	$A = 2$ –4, 16–24	17	$5 \cdot 10^8$	$1.3 \cdot 10^{-6}$

Parameter	median	68% credible region
$\tilde{C}_{1S0pp}$	-0.343	[-0.360, -0.327]
$\tilde{C}_{1S0np}$	-0.339	[-0.352, -0.328]
$\tilde{C}_{1S0nn}$	-0.337	[-0.349, -0.327]
$\tilde{C}_{3S1}$	-0.258	[-0.272, -0.245]
$C_{1S0}$	2.502	[2.377, 2.785]
$C_{3P0}$	1.343	[1.217, 1.600]
$C_{1P1}$	-0.273	[-0.600, -0.115]
$C_{3P1}$	-1.074	[-1.199, -0.834]
$C_{3S1}$	0.982	[0.803, 1.160]
$C_{E1}$	0.437	[0.358, 0.512]
$C_{3P2}$	-0.920	[-1.032, -0.809]
$c_1$	-0.740	[-0.760, -0.721]
$c_2$	-0.494	[-0.645, -0.347]
$c_3$	-0.645	[-0.841, -0.456]
$c_4$	0.958	[0.861, 1.056]
$c_D$	-0.460	[-1.955, 0.175]
$c_E$	-0.107	[-0.471, 0.196]

**Extended Data Table 3** | Medians and 68% credible regions (highest-density intervals) from the Bayesian posterior pdf of  $\chi$ EFT model parameters obtained with MCMC sampling as described in the text.

Parameter	median	68% credible region
$\tilde{C}_{1S0pp}$	-0.343	[-0.360, -0.327]
$\tilde{C}_{1S0np}$	-0.339	[-0.352, -0.328]
$\tilde{C}_{1S0nn}$	-0.337	[-0.349, -0.327]
$\tilde{C}_{3S1}$	-0.258	[-0.272, -0.245]
$C_{1S0}$	2.502	[2.377, 2.785]
$C_{3P0}$	1.343	[1.217, 1.600]
$C_{1P1}$	-0.273	[-0.600, -0.115]
$C_{3P1}$	-1.074	[-1.199, -0.834]
$C_{3S1}$	0.982	[0.803, 1.160]
$C_{E1}$	0.437	[0.358, 0.512]
$C_{3P2}$	-0.920	[-1.032, -0.809]
$c_1$	-0.740	[-0.760, -0.721]
$c_2$	-0.494	[-0.645, -0.347]
$c_3$	-0.645	[-0.841, -0.456]
$c_4$	0.958	[0.861, 1.056]
$c_D$	-0.460	[-1.955, 0.175]
$c_E$	-0.107	[-0.471, 0.196]



**Extended Data Fig. 7 | Posterior predictive distributions for  $^{16,22,24}\text{O}$ .** MCMC samples of the posterior predictive distribution for selected oxygen observables. The black (maroon) histogram shows results obtained with an uncorrelated, Gaussian likelihood (including a discrete probability  $p(E_{np,1S0} > 0|\theta) = 1$ ). The red histogram illustrates a low-statistics sample. The 68% credible regions and the medians are indicated by dashed lines on the diagonal, while the solid, vertical grey (blue) lines show the experimental target (prediction with the  $\Delta\text{NNLO}_{\text{GO}}$ (394) interaction).