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Parametrization of the Coulomb interaction matrix with point-group symmetry

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Motivation: beyond spherical symmetry

Coulomb integrals are relevant for spectroscopies and *ab initio* methods on strongly correlated materials

$$U_{ijtu} = \int d\vec{r} d\vec{r}' \phi_i(\vec{r})^* \phi_j(\vec{r}')^* U(\vec{r}, \vec{r}') \phi_t(\vec{r}) \phi_u(\vec{r}')$$

ϕ_i : a one-electron wave function

State of the art: Slater parametrization (1930), derived for $1/r$ potentials.

$$U_{ijtu} = \sum_k c_k(ij, tu) R^k(ij, tu)$$

→ but: exact **only** in spherical $SO(3)$ symmetry

Step 1: point-group symmetry

Let ϕ_i, \dots, ϕ_u transform as given irreducible representations (irreps) α, \dots, δ of the point group G . We diagonalize $U^{\alpha\beta\gamma\delta}$ in the basis of irreps $\{\eta\}$ of G (Schur's lemma).

$$U^{\alpha\beta\gamma\delta} = [C^{\alpha\beta, \eta}]^{-1} \begin{pmatrix} I^{\eta_1} & & \\ & I^{\eta_2} & \\ & & I^{\eta_3} \end{pmatrix} [C^{\gamma\delta, \eta}]$$

The Clebsch-Gordan coefficients $C^{\alpha\beta, \eta}$ couple the direct product of irreps $\alpha \otimes \beta \rightarrow \eta$

The I^η are G -invariant and independent of the basis of U .

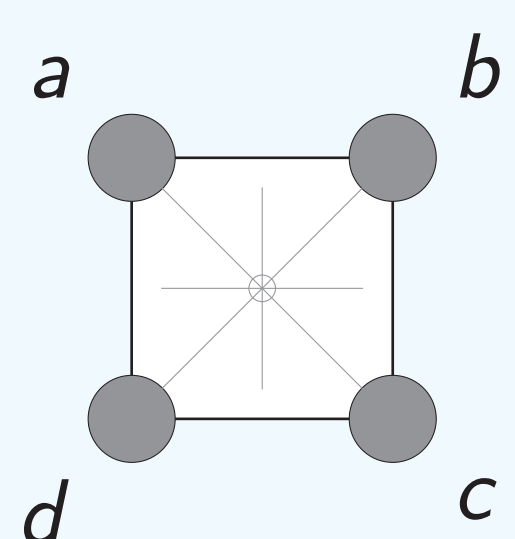
$$I^{\alpha\beta\gamma\delta, \eta} = \frac{1}{[\eta]} \sum_{e=1}^{[\eta]} C^{\alpha\beta, \eta} U^{\alpha\beta\gamma\delta} [C^{\gamma\delta, \eta}]^{-1}$$

→ exact parametrization of $U^{\alpha\beta\gamma\delta}$ for any point group

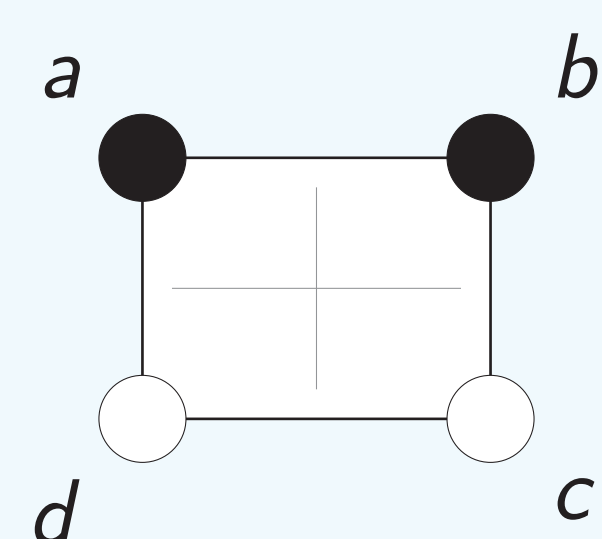
Step 2: permutation symmetry

The number of parameters can be reduced further by considering the invariance of U_{ijtu} under permutation of the wave functions.

The permutation group \mathcal{P} differs for real and complex wave functions.



real case:
 D_4 group



non-real case:
 $m'm2'$ group

Projection of the invariants onto the fully-symmetric irrep A_1 of the permutation group:

$$\langle I^\eta \rangle \stackrel{\text{def}}{=} \frac{1}{|\mathcal{P}|} \sum_{\sigma_i \in \mathcal{P}} \sigma_i \triangleright I^\eta = M_{\eta\phi} I^\phi$$

→ minimal set of independent parameters

Structural symmetry breaking

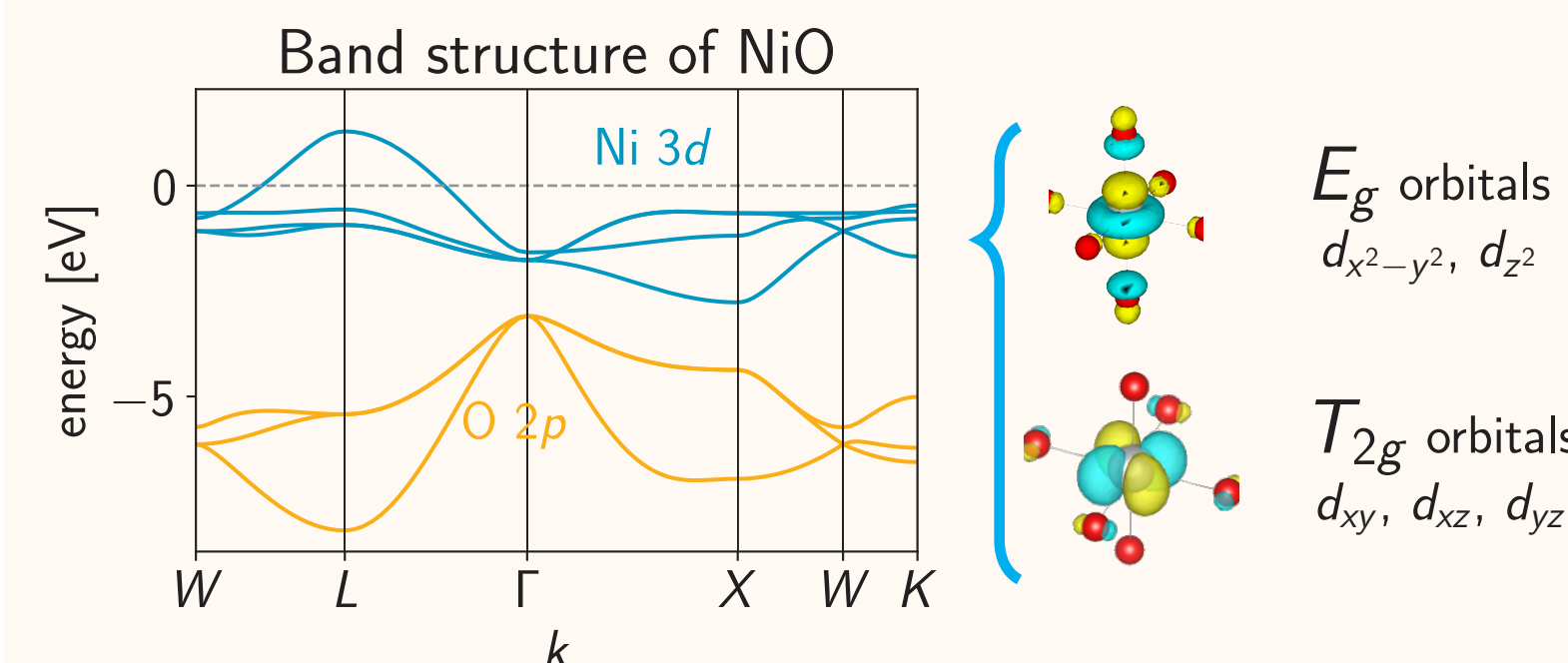
It corresponds to the subduction from the initial point group \mathcal{G} (eg. $SO(3)$) to one of its subgroups G . We relate the \mathcal{G} invariants to the G invariants using isoscalar factors.

$$C_{\alpha\beta, \eta e}^{l_1 l_2, \ell} = \begin{pmatrix} l_1 & l_2 & \ell \\ \alpha & \beta & \eta \end{pmatrix} C_{ab, e}^{\alpha\beta, \eta}$$

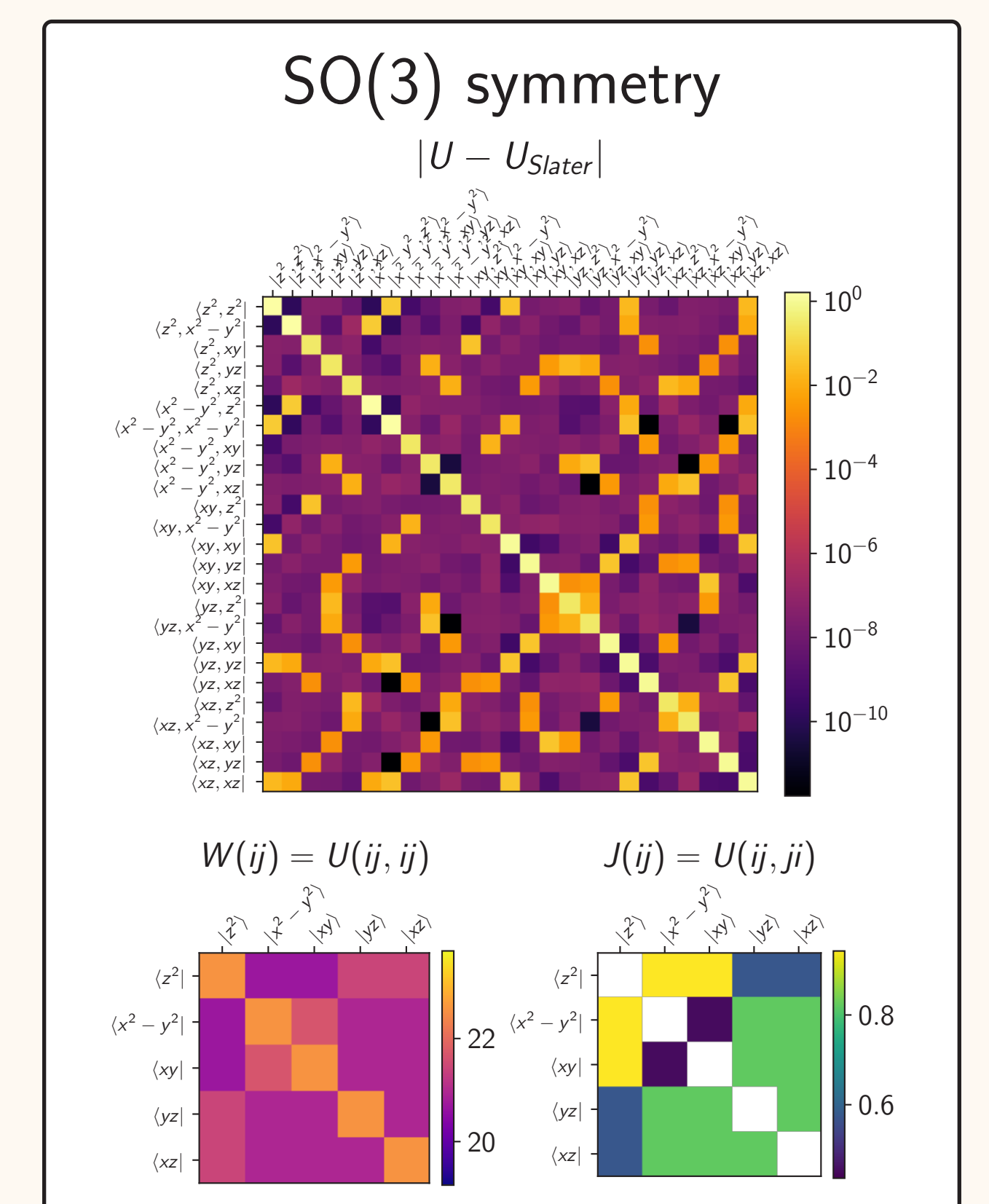
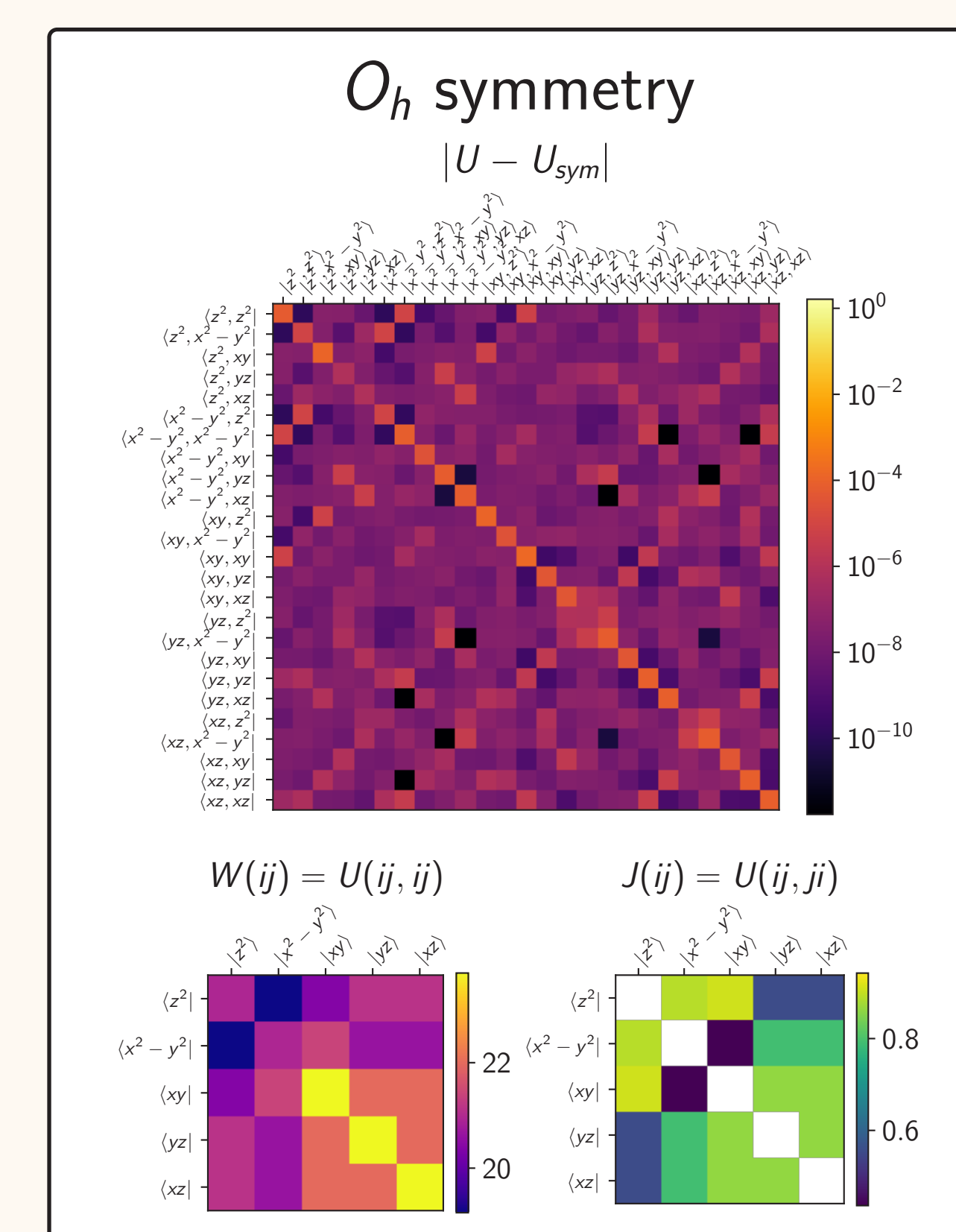
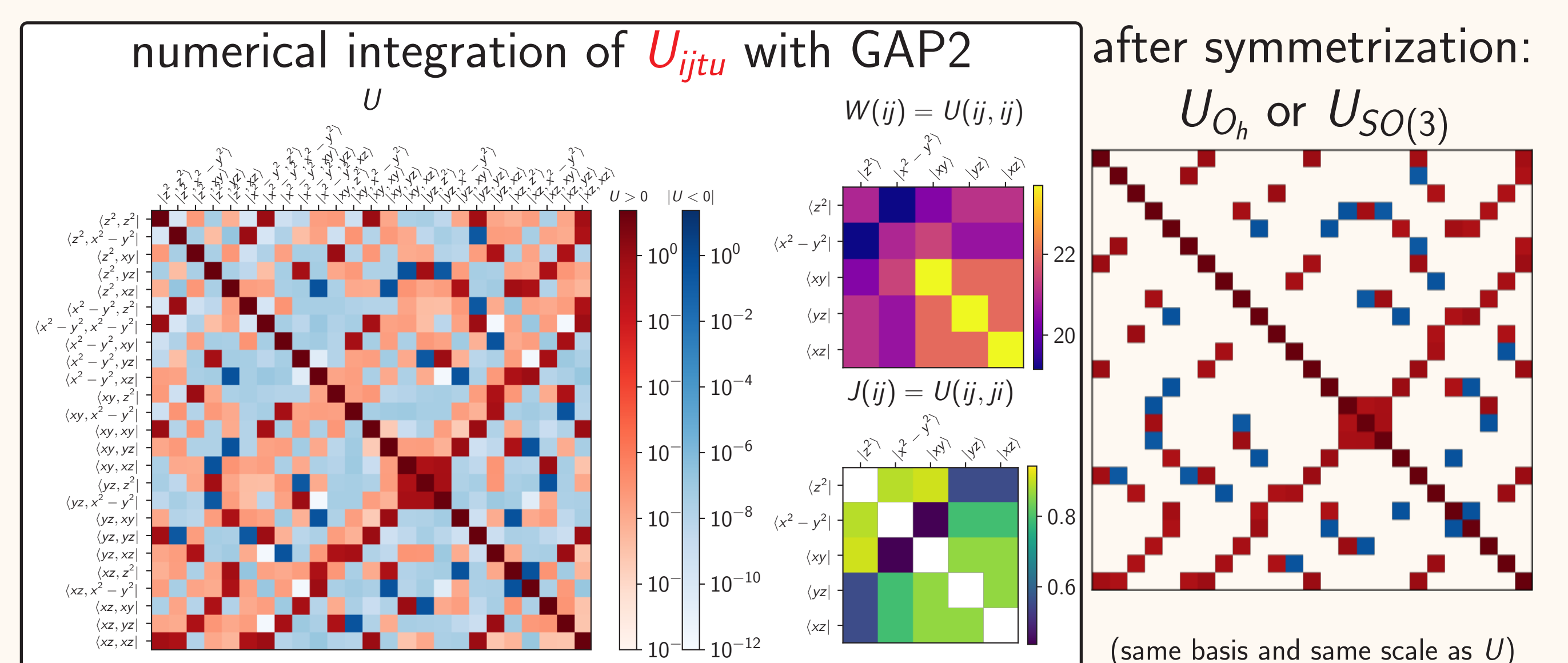
$$I^{\eta(l_1 \alpha l_2 \beta l_3 \gamma l_4 \delta, \eta)} = \sum_{\ell} \begin{pmatrix} l_1 & l_2 & \ell \\ \alpha & \beta & \eta \end{pmatrix} \begin{pmatrix} l_3 & l_4 & \ell \\ \gamma & \delta & \eta \end{pmatrix}^* I^{\eta(l_1 l_2 l_3 l_4, \ell)}$$

NiO, a 3d shell in octahedral O_h symmetry

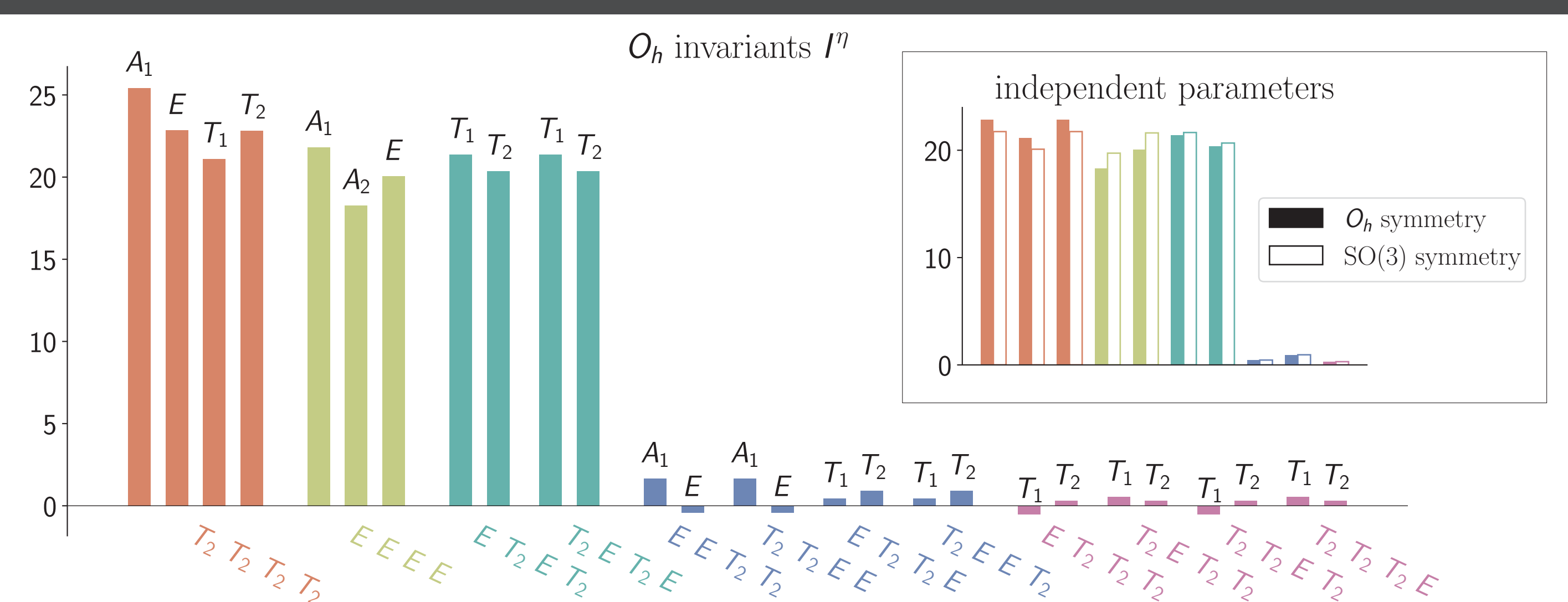
All values are in eV, for the *bare* Coulomb interaction. Also applicable to screened interactions (eg. via cRPA).



Wannier functions of the Ni 3d shell: a localized and symmetry-adapted basis set for the interacting subspace



Oh invariants



Conclusion and Outlook

▶ $U \approx \sum_k c_k R^k \rightarrow U = \sum_{\eta} c_{\eta} I^{\eta}$ for any point group

▶ in progress: DMFT calculations with point-group symmetrized interaction

Miscellaneous

▶ on arXiv: 2306.10186; accepted for publication in PRB

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