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► **To cite this version:**

Sylvain Picaud, Arnaud Desmedt, Ludovic Martin-Gondre, Victoire Meko-Fotso. Molecular simulations of mixed clathrate hydrates including ionic species. European Conference on Gas Hydrate - ECGH 2024, Jun 2024, Trieste, Italy. pp.72. hal-04913733

**HAL Id: hal-04913733**

**<https://hal.science/hal-04913733v1>**

Submitted on 27 Jan 2025

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## Molecular simulations of mixed clathrate hydrates including ionic species

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The world faces a dual challenge of climate change driven by greenhouse gas emissions and the finite nature of fossil fuels. Hydrogen turns out to be an alternative to solve this problem since its combustion leads to water and energy. However, hydrogen storage and safe transportation remains a challenging task. Among all proposed hydrogen storage materials, storage in clathrate hydrates constitutes an attractive hosting environment [1]. In this work, we initially studied the properties of neutral systems presenting interesting characteristics for hydrogen storage: N<sub>2</sub> gas hydrate for its storage capacity and Xe gas hydrate for its thermodynamic stability in soft conditions. In addition, a second promoter is considered in order to improve the H<sub>2</sub> diffusion. Indeed, ionic species (such as HClO<sub>4</sub>) can modify the dynamics properties of the aqueous network and help the H<sub>2</sub> inter-cage diffusion [2]. The properties of mixed clathrate hydrates are determined by Density Functional Theory (DFT) simulations using the Vienna Ab initio Simulation Package (VASP) and considering two functionals. Initially, the structural properties of mixed hydrates are studied. Then, the thermodynamic properties of clathrates are evaluated with a convex hull approach in order to extract effects of pressure and acid composition on stability.

[1] Gupta A., Baron G.V., Perreault P., Lenaerts S., Ciocarlan R-G, Cool P., Mileo P.G.M., Rogge S., Van Speybroeck V., Watson G., Van der Voort P., Houlléberghs M., Breynaert E., Martens J., Denayer J.F.M., **2021**. Hydrogen Clathrates: Next Generation Hydrogen Storage Materials. *Energy Storage Mat.* 41, 69-107.

[2] Nguyen T.T., Petuya C., Talaga D., Desmedt A., **2020**. Promoting the Insertion of Molecular Hydrogen in Tetrahydrofuran Hydrate With the Help of Acidic Additives. *Frontiers in Chemistry* 8, 550862.