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Hydrogen storage in charge compensated organic molecular crystals MINA YOON, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany and Oak Ridge National Laboratory, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — We propose charge compensated organic molecular crystals as a promising class of materials for hydrogen storage. Using quantum mechanical first-principles calculations based on numerical atom-centered orbitals as all-electron basis functions [1] we study the basic structural properties of molecular crystals consisting of parallel sheets of cations and anions (such as DMPH and TCNQ) stacked alternatingly. The long range dispersion interactions between the cations and anions, which are important for the stability of the crystals, were studied and compared using various DFT xc functionals, semi-empirical approach [2], and Møller-Plesset perturbation theory. The molecular configuration causes accumulation of electrons at acceptors and depletion at donors, which results in finite dipolar fields. Our study indicates that these fields make it possible to use charge compensated organic molecular crystals for hydrogen storage.

[1] V. Blum *et al.*, FHI ab initio molecular simulations (FHI-aims) project.
[2] A. Tkatchenko and M. Scheffler, to be published.

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