

Abstract Submitted
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Zero and finite temperature adsorption energies in zeolites: A random phase approximation study¹ ANANT DIXIT, MICHAEL BADAWI, University of Lorraine (France), TOMAS BUCKO, Comenius University in Bratislava and Slovak Academy of Sciences (Slovakia), SEBASTIEN LEBEGUE, JANOS ANGYAN, DARIO ROCCA, University of Lorraine and CNRS (France) — Zeolites are widely used in industry as sorbents and catalysts due to their porous structures that can host various ions and molecules [1]. Adsorption of molecules in zeolites is typically determined by van der Waals (vdW) forces. This represents a challenge for ab-initio calculations, since semi-local approximations based on the density functional theory (DFT) fail to include vdW interactions. The random phase approximation (RPA) is an ab-initio scheme to build a fully non-local correlation functional that accurately captures vdW forces. The RPA can today describe realistic systems with a few hundreds of electrons and generate accurate benchmarks. Using the RPA as implemented in Refs. 2-3 we compute adsorption energies of methane and carbon dioxide in siliceous chabazite at 0 K. To evaluate temperature effects on the interaction energy we average over multiple configurations generated by molecular-dynamics simulations at 300 K. These results are compared with those obtained using DFT approximations with semi-empirical corrections.[1] S. Auerbach, K. Carrado, P. Dutta, Handbook of Zeolite Science and Technology, CRC Press (2003) [2] D. Rocca, J. Chem. Phys. 140, 18A501 (2014) [3] A. Dixit, J. Angyan, D. Rocca, J. Chem. Phys. 145, 104105 (2016)

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