Adsorption of CO_2 on modified Fe_3O_4 surfaces studied by density-functional theory

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In recent years, Fe_3O_4 (magnetite) represents a versatile oxide material due to many industrial applications [1-2]. The Atomic level understanding on the interaction of H_2O and other molecules on Fe_3O_4 surfaces have been studied and reported. However, the CO_2 adsorption and activation are still topic of current research [3]. The capture and storage of CO_2 plays an important role for the greenhouse effect and carbon recycling.

This work reports results on periodic models of adsorbed CO_2 on various modified Fe_3O_4 surfaces. As an initial stage of CO_2 activation study, adsorption thermodynamics of different CO_2 coverage up to 2 ML is studied. We employ density-functional theory using the Perdew, Burke, Ernzerhof [4] gradient-corrected exchange-correlation functional including a correction for the Fe 3d levels by an onsite Hubbard-type U parameter. This approach was shown to perform accurately for the description of important bulk properties [5].

References:
[1] Smit, E. de; Weckhuysen, B. Chem. Soc. Rev. **2008**, 37, 2758.
[2] Ratnasamy, C. Catal. Rev. **2009**, 51, 325.
[3] Pavelect J.; Diebold U.; Parkinson G. S. J. Chem. Phys. **2017**, 146, 014701
[4] Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. **1996**, 77, 3865.
[5] Li, X.; Paier, J. J. Phys. Chem. C **2016**, 120, 1056.