Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

A new DFT approach to model small polarons in oxides with proper account for long-range polarization[1] SEBASTIAN KOKOTT, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society, THEORY DEPARTMENT TEAM — In this work, we address two important challenges in the DFT description of small polarons (excess charges localized within one unit cell): sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO_2 on the XC functional. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a finite-size correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allowed us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, Phys. Rev. B **92**, 075202 (2015); [2] S.I. Pekar, Zh. Eksp. Teor. Fiz. **16**, 335 (1946).

[1]partially supported by UniCat (Deutsche Forschungsgemeinschaft)

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Date submitted: 07 Nov 2016 Electronic form version 1.4