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**First-principles Evidence for Intermediate Hole Polarons in ZnO**
HONGHUI SHANG, CHRISTIAN CARBOGNO, Fritz-Haber-Institut der MPG, Berlin, DE, PATRICK RINKE, Fritz-Haber-Institut der MPG, Berlin, DE and Aalto University, Helsinki, Fi, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE, HIKMET SEZEN, FABIAN BEBENSEE, CHENGWU YANG, MARIA BUCHHOLZ, ALEXEI NEFEDOV, STEFAN HEISSLER, CHRISTOF WÖLL, Karlsruhe Institute of Technology, Karlsruhe, DE — We performed density functional theory calculations at the hybrid-functional level (HSE06) to investigate the nature of the polaronic states in ZnO. Our calculations confirm that neither small (i.e., strong coupling) electron nor hole polarons are stable in ZnO, in agreement with previous studies [1]. The binding energy of large polarons (i.e., weak coupling) was determined by evaluating the renormalization of the band edges due to the zero-point motion of the atoms [2]. However, for intermediate polarons at intermediate coupling strength, the harmonic approximation breaks down, and there is currently no first-principle theory. We use the HSE06 effective masses to calculate the Fröhlich coupling constants $\alpha$. Feynman's path integral technique then yields an intermediate hole polaron, whose binding energy of 245 meV and associated peaks in the optical absorption spectrum are consistent with infrared reflection absorption spectroscopy.

[1] J. B. Varley *et al.*, Phys. Rev. B **85**, 081109(R)(2012).
[2] G. Antonius *et al.*, Phys. Rev. Lett. **112**, 215501 (2014)

Honghui Shang
Fritz-Haber-Institut der MPG, Berlin

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