Abstract Submitted
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Electronic structure and van der Waals interactions in the stability and mobility of point defects in semiconductors WANG GAO, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT TEAM — Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV. Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can accurately describe both the formation energies and migration barriers of point defects. The inclusion of vdW interactions largely changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW energy plays an increasingly larger role [2]. [1] G. X. Zhang *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012). [2] W. Gao *et al.*, PRL **111**, 045501 (2013).

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