Abstract Submitted
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Improved metallic surface properties using a new van der Waals density functional ABHIRUP PATRA, JIANWEI SUN[1], JEFFERSON BATES, JOHN P. PERDEW, Department of Physics, Temple University,Philadelphia, Pennsylvania — An incorrect description of van der Waals (vdW) interactions for different problems using popular density functional theory (DFT) is found in many cases, especially where long-range van der Waals interactions are present. Metallic surfaces are such systems. Physical properties of surfaces such as surface energy and work function can be affected by the long-range van der Waals interaction present at the surface barrier. In this work we explore the performance of the new vdW-corrected non-local density functional SCAN+rVV10[1] for such surfaces. We find that, when the new meta-GGA functional SCAN is combined with the non-local rVV10 method, it can not only give a better description of the van der Waals interaction in molecules and layered materials, but can be equally used as a more versatile competitor of LDA for metal surfaces. 1.Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation, H. Peng, Z. Yang, J. P. Perdew, J. Sun, Phys. Rev. X 6, 041005 (2016). Acknowledgments: NSF under DMR-1305135, CNS-09-5884, and by DOE under DE-SC0012575, DE-AC02-05CH11231

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