Abstract Submitted
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Toward an accurate and practical description of Xe/Cu(111) physisorption GAROLD MURDACHAEW, SISSA, STEFANO DE GIRONCOLI, SISSA and DEMOCRITOS, PATRICK HUANG, EMILY CARTER, Princeton University, GIACINTO SCOLES, SISSA and Princeton University — The physisorption of rare gases on metal surfaces has often been described by density functional theory. However, standard DFT has shown very limited success due to its well-known shortcomings when applied to weak interactions. A possible approach which at least includes the relevant missing physics is to use a blend of "corrected" DFT coupled with a damped-dispersion interaction. Alternatively, one may model the surface by a cluster since it is possible to apply highly accurate quantum chemical methods to small clusters. Unfortunately, cluster model approximations do not give a good description of the physisorption process on the surface. In particular, the site preference of Xe/Cu(111) physisorption as given by cluster models is qualitatively incorrect. For this reason, an approach which better simulates the surface is required. Some recent results obtained using the embedded cluster approach of E. A. Carter, P. Huang, and coworkers [P. Huang and E. A. Carter, J. Chem. Phys. **125**, 084102 (2006)] will be presented.

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