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A density functional theory study of the benzene-water complex

SHEN LI, VALENTINO COOPER, Department of Physics and Astronomy, Rutgers, The State University of New Jersey, T. THONHAUSER, Department of Physics and Astronomy, Rutgers The State University of New Jersey and Department of Materials Science and Engineering, MIT, AARON PUZDER, Department of Physics and Astronomy, Rutgers, The State University of New Jersey and Lawrence Livermore National Laboratory, DAVID LANGRETH, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — We calculated the intermolecular interaction of the benzene-water complex using real-space pseudopotential density functional theory with a van der Waals density functional (vdW-DF). Developed recently, vdW-DF has been applied to a number of van der Waals complexes with promising results. Our results for the intermolecular potential energy surface between benzene and a water molecule clearly show a stable configuration with the water molecule standing above the benzene with one or both of the H atoms pointing toward the benzene plane, as predicted by previous studies. However, when the water molecule is pulled outside the perimeter of the benzene ring, the configuration of the complex becomes unstable with the water molecule attaching in a saddle point configuration to the rim of the benzene with its O atom adjacent to a benzene H. The results for ground state structure are compared with available experiments and quantum chemical calculations.

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