Nature of Interaction of Graphene with Ag, Au, Pd Metals

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We studied the adsorption of Ag, Au, and Pd atoms on benzene, coronene and graphene using post Hartee-Fock wave-function theory (CCSD(T), MP2) and density functional theory (M06-2X, DFT-D3, PBE, vdW-DF) methods. The binding energies calculated by CCSD(T) method for benzene...M (M=Pd, Au, Ag) complexes are 19.7, 4.2, and 2.3 kcal/mol, respectively. The nature of binding of the three metals is different. Silver binds predominantly through dispersion interactions, the binding of palladium has a covalent character, and the binding of gold involves a subtle combination of charge transfer and dispersion interactions, as well as relativistic effects. These effects can be reproduced in plane-wave density functional theory calculations by including a fraction of the exact exchange and a nonempirical (vdW-DF) van der Waals correction (EE+vdW). The calculated EE+vdW energies agree well with the benchmark CCSD(T) energies for benzene...M complexes. The EE+vdW binding energies for the graphene...M (M=Pd, Au, Ag) complexes are 17.4, 5.6 and 4.3 kcal/mol, respectively. The interaction of larger metal clusters will also be discussed.

References

[1] Granatier J, Lazar P, Otyepka M, Hobza P J. Chem. Theory Comput., **7** (2011) 3743.