Abstract Submitted
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Theoretical DFT Study of Homonuclear and Binary Transition-Metal Dimers[1] ALVARO POSADA-AMARILLAS, Dept. de Investigacion en Fisica, Universidad de Sonora, ALVARO POSADA-BORBON, Dept. de Fisica, Universidad de Sonora — A DFT study of homonuclear, and heteronuclear Pd-M, Pt-M (M=Cu, Ag, Au, Ni) and Pt-Pd neutral dimers is presented using different XC functionals and basis sets. Bond length and vibrational frequencies were determined for ground state configurations. Doublet and triplet states were obtained for heteronuclear dimers while dissociation energy exhibits unambiguous dependency on the HF exchange term. Electronic configurations were determined for Pd-Ag ($^2\Sigma$) and Pt-Ni ($^3\Sigma$) dimers. Hybrid functionals provide results in close agreement with experimental data for Pt-Ni, Pt-Pd, and Pd-Ni dimers. The hybrid mPW1PW91 functional predicts a dissociation energy value for Pt-Cu dimer of about 3.3 eV, consistent with experimental information. Overall PBE and B3PW91 are reliable functionals to predict bond lengths and harmonic frequencies of heteronuclear dimers.

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