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Single, Double and Triple Intercluster Bonds. Analyses of $M_2Au_{36}(SR)_{24}$ (M=Au, Pd, Pt) as 14-, 12- and 10-ve Superatomic Molecules

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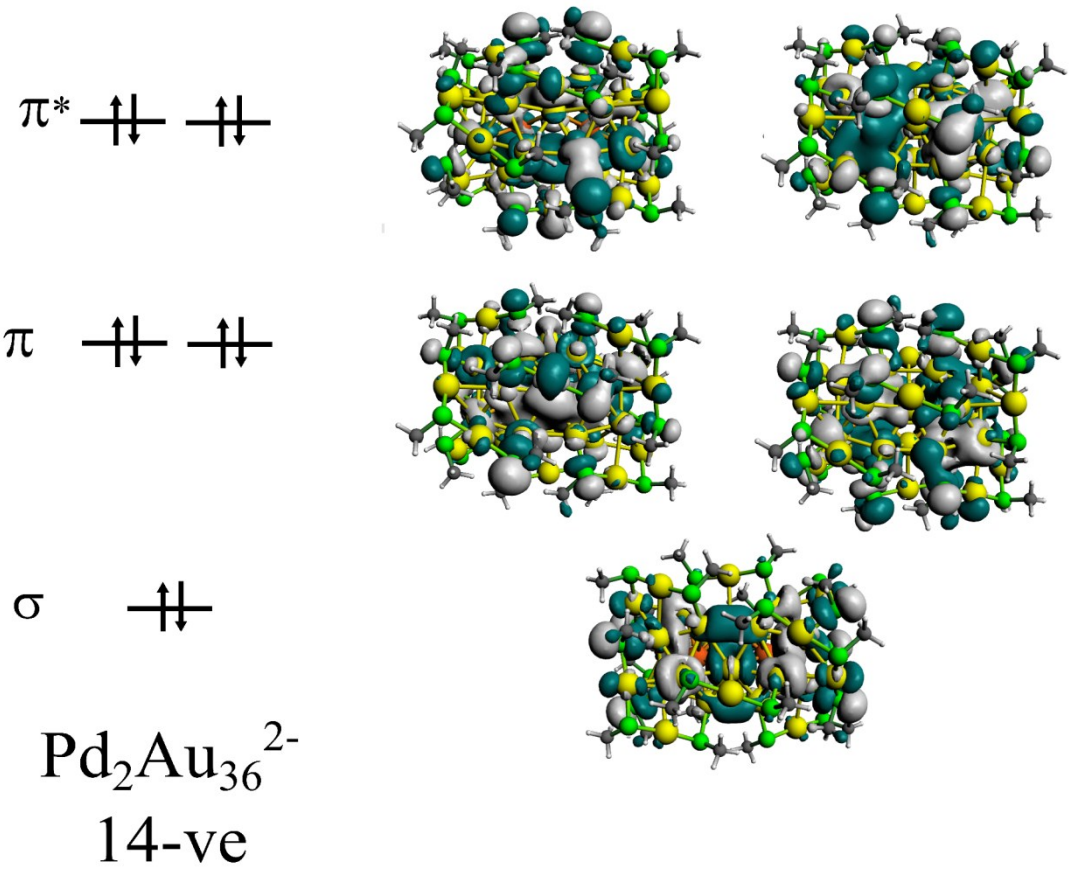

Figure S1. Molecular orbitals resembling to σ, π and π* combinations from the 1P+1P interaction for the representative $Pd_2Au_{36}^{2-}$ biicosahedral cluster.

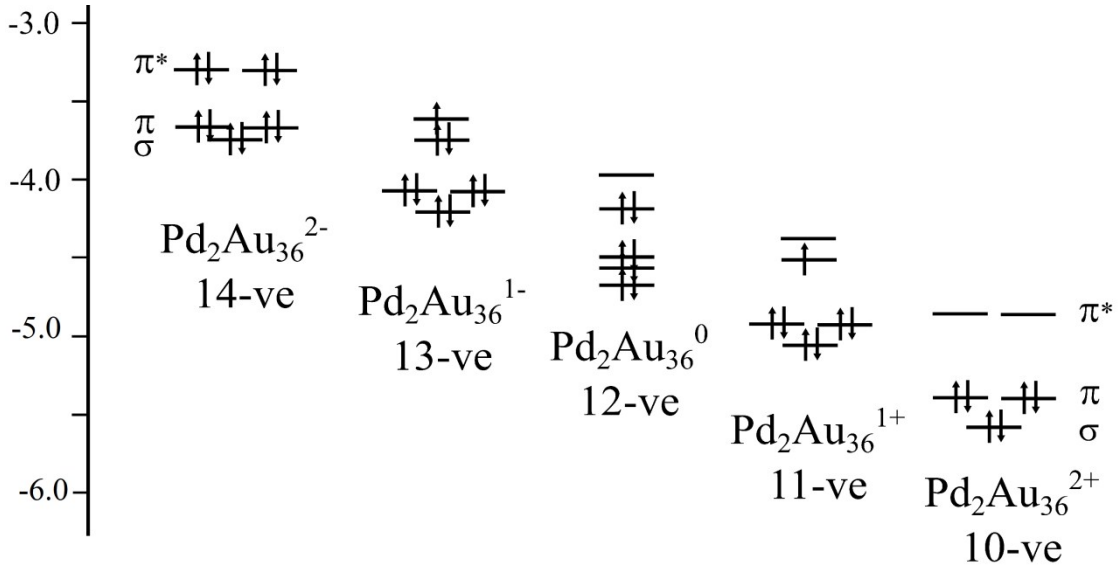

Figure S2. Molecular orbitals levels resembling to σ, π and π* combinations from the 1P+1P interaction for the representative Pd_2Au_{36} biicosahedral cluster ranging from -2 to +2 charge states. Energy scale in e. Calculated at the TZ2P-PBE/ZORA-SR COSMO (dichloromethane) level.