

Supporting Information

Hot Carrier Creation in a Nanoparticle Dimer-Molecule Composite

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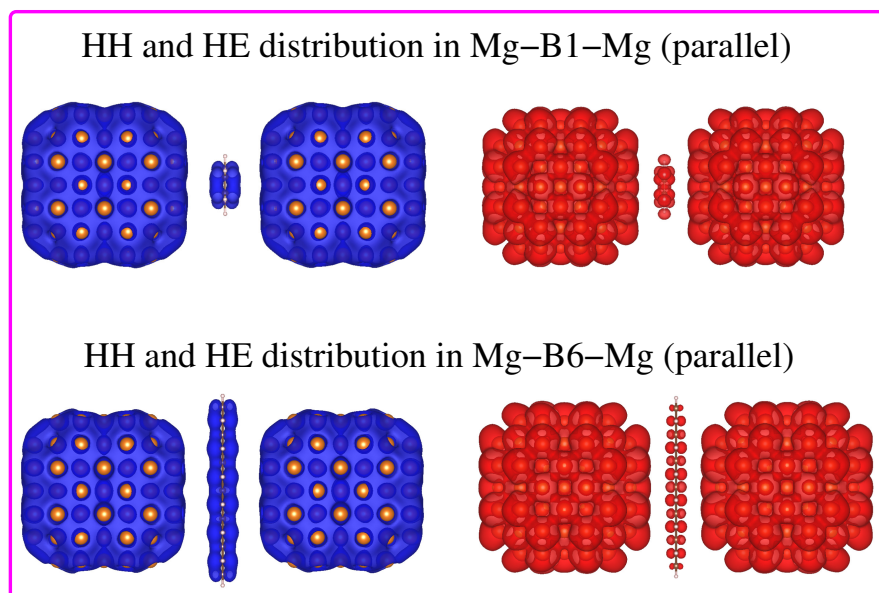


Figure S1: hot carrier distribution of Mg-B1-Mg (top) and Mg-B6-Mg (down) with parallel configuration of PAH molecules.

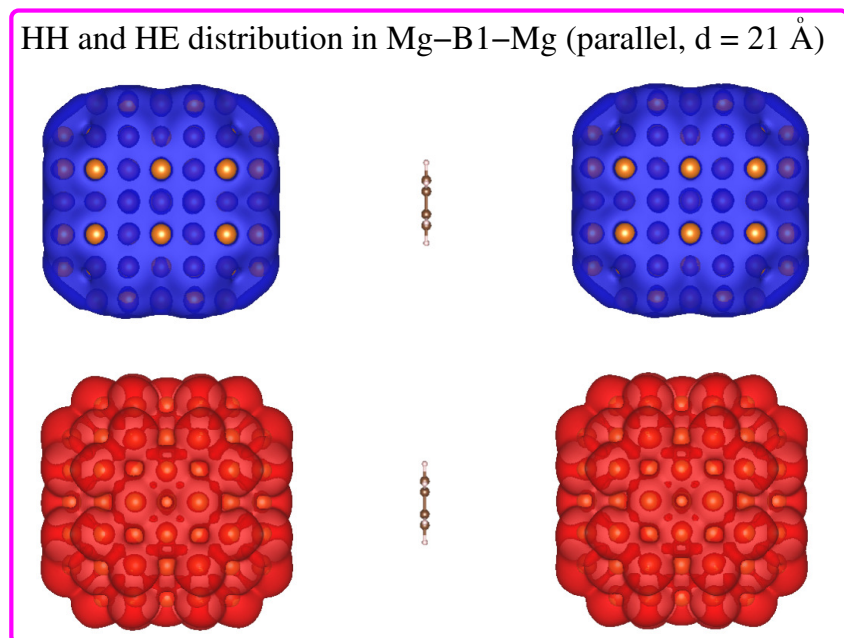


Figure S2: hot carrier distribution of Mg-B1-Mg parallel configuration with a large interparticle gap value of 21 \AA .

Mg-Adenine-Mg

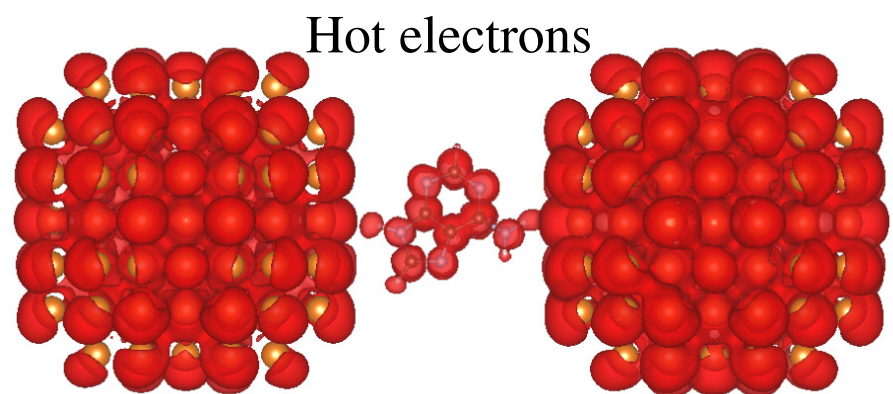
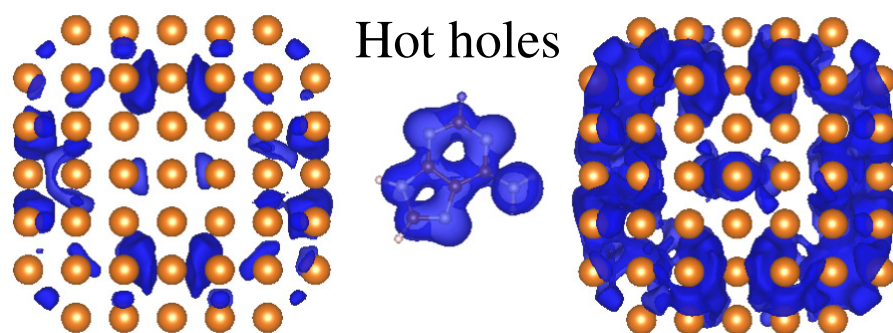


Figure S3: hot carrier distribution of Mg-Adenine-Mg.

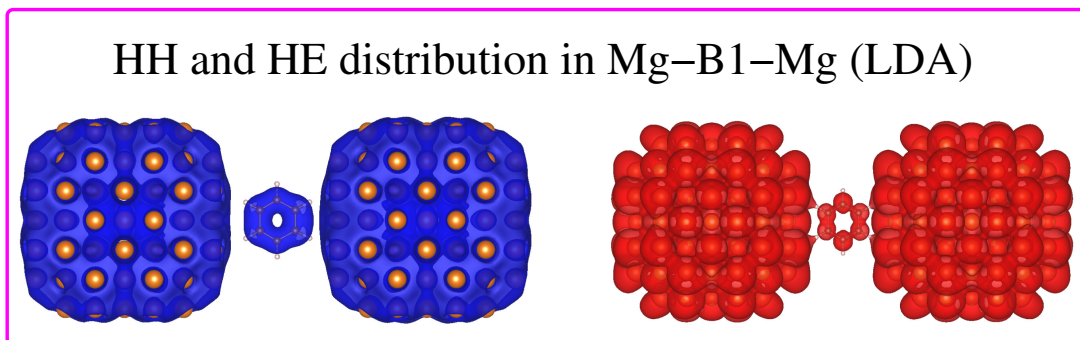
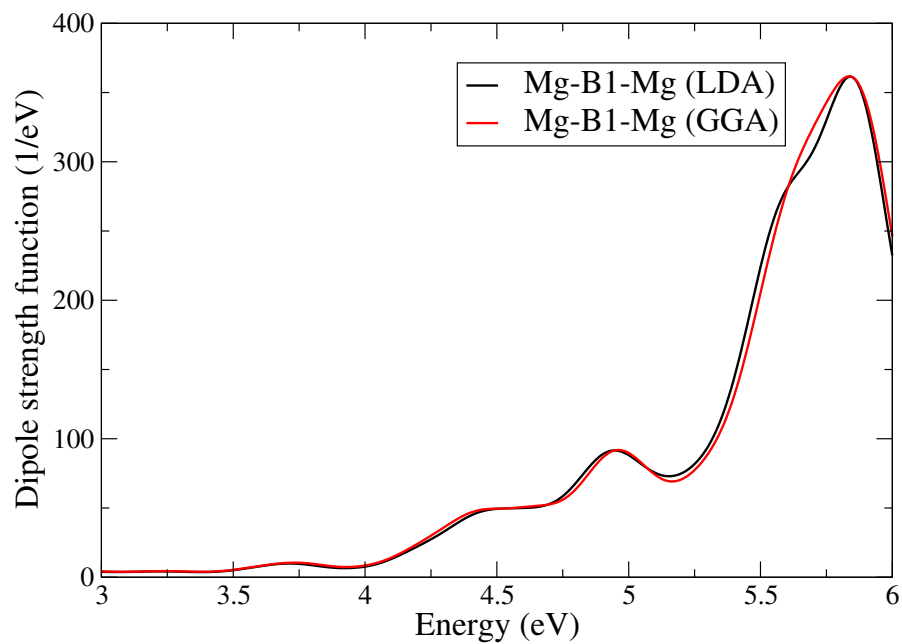


Figure S4 illustrates: at the top, a comparison of photabsorption using LDA and GGA functionals, and at the bottom, the distribution of hot carriers in Mg-Adenine-Mg.