PL-12

IN-SILICO DESIGNING OF FUNCTIONAL MATERIALS

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Abstract. The functionalities depends on the electronic energy levels of the materials concerned and therefore understanding the electronic structure is of paramount importance in designing such materials. By using density-functional tight-binding method (DFTB) we herein discussed the pathways for improving the photovoltaic efficiency of the tetra phenyl porphyrin(TPP)-phosphorene antidot lattice(PAL) nanocomposites. The photovoltaic performance of the composite reaches a maximum value when TPP is functionalized by -NH2 group and the edge of PAL is functionalized by -CN group. We also discussed the role of chalcogen ligands on the exciton relaxation dynamics of chalcogenol functionalized CdSe QD by using non-adiabatic molecular dynamics simulation (NAMD) coupled with the DFTB method.

References

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