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Optical Properties of Molecules and Molecular Aggregates Adsorbed on Solid Surfaces. First Principle Study. ALEXANDER GAVRILENKO, MIKHAIL NOGINOV, CARL BONNER, VLADIMIR GAVRILENKO, Center of Materials Research, Norfolk State University, Norfolk VA 23504 — Equilibrium atomic geometries of Ferrocene and Rhodamine 6G (R6G) dye molecules adsorbed on Si(111) and Ag(111) surfaces respectively are studied using density functional theory. Equilibrium atomic geometries are obtained through total energy minimization method. Electron energy structure and optical properties are calculated using generalized gradient approximation method with *ab initio* pseudopotentials. Modifications of electronic surface structures of Ag(111) and Si(111) caused by the adsorption of molecules as well as charge transfer between molecules and solids are studied. Red or blue shifts of optical absorption spectra of R6G dye molecules after aggregation in J- or H-dimmers respectively are predicted. Calculated optical absorption spectra are interpreted in terms of inter-molecular and molecular-solid interactions. Results of the calculations are discussed in comparison with experimental data.

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