Theoretical analysis of molecules and clusters attached to bulk conducting, semiconducting and insulating materials

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1. The physical, chemical, and electrical characteristics at bulk-molecule and bulk-cluster interfaces are studied, where the bulk material, which can be a conducting, semiconducting or insulating material, can be attached to any molecule or cluster. The molecule, cluster, and their neighborhood atoms, as well as the effects of the extended and continuum nature of the bulk are considered through the use of molecular and extended ab initio procedures interconnected by a Green function formalism to account for the interfacial characteristics. A systematic evaluation of several molecules, clusters, and bulk materials is performed to determine their junction electrical characteristics. We characterize the molecule or cluster using our combined density functional-Green function approach. In typical experiments of electron conduction for instance, molecules are attached to one of the contacts by self-assembling, and by metal vapor deposition on the other contact. Thus we extend the molecule and their ions are with few atoms from the bulk at each end and fully optimized the geometry using several levels of theory. The bulk material structure is also fully optimized using a similar procedure specialized for periodic systems.