

First-principles Study of Metal Impurity Induced Electronic Structure Change in Pentacene

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Abstract

Organic semiconductors have received much attention due to their potential applications in a variety of optical and electronic devices such as light emitting diodes and field effect transistors. The potential advantages of using organic semiconductors include low cost, low power consumption and flexible substrate roll-to-roll processing, which are not readily accessible by conventional silicon based microelectronics. Among the large selection of organic semiconducting materials, pentacene ($C_{22}H_{14}$) has attracted great interests due to its high carrier mobility as high as $35 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ [1], exceeding that of amorphous silicon.

However, to fully exploit the intrinsic high carrier mobility of pentacene and obtain optimal device performance, it is crucially important to have an efficient charge transport process across the metal-organic interfaces. Typical organic field effect transistors consist of a layer of pentacene film deposited on an insulator, with metal source and drain electrode on top. At the metal-organic interface where charge injection takes place, due complex physical and chemical processes (such as bond formation, impurity diffusion, charge transfer or electronic polarization) physical properties of the pentacene film may no longer resemble its intrinsic properties. For example, it has been demonstrated experimentally that hot metal impurity atoms may diffuse into the weakly bonded pentacene network and strongly influence its conductive properties [2]. Despite the significant experimental and theoretical efforts devoted into the research of interfacial properties, a detailed atomistic understanding of interactions at metal/pentacene interface is still lacking.

In this study, we report the first-principles investigation of binding properties of six different metal atoms (La, Ti, Ru, Ni, Au, and Pd) to pentacene molecule and the induced electronic structure changes. It has previously been recognized that the interface energy alignment depends on the charge transfer and the resulting interface dipole [3]. We show that the diffusion of metal atoms into the pentacene film and its interaction with pentacene molecules further modify the injection barrier by wavefunction hybridization.

Depending on the interaction strength and degree of orbital hybridization between the metal atom and pentacene molecule, the metal-pentacene complex shows distinctive characteristics and can be grouped into three categories: i) weak hybridization and negligible perturbation to intrinsic pentacene electronic structure (Pd); ii) hybridization of between metal d-orbitals and π -electrons leading to the formation of mid gap states (Au, Ni, Ru); iii) strong interaction of the metal impurity and pentacene completely altering the intrinsic pentacene electronic structure (La, Ti). Through the orbital and band structure analysis, it is revealed that metal d-orbital plays an important role in the metal interaction with pentacene's π -electron. The implication of metal impurity induced electronic structure change is discussed in the context of carrier transport across the interface.

References

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