527d Electron Transport on Metal-Molecule-Semiconductor Interfaces

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The formation of Schottky barriers in metal-semiconductor interfaces represents a non-totally understood phenomenon; this effect deters the injection of electrons to any semiconductor-based integrated circuit. Functionalized molecules assembled between the metal and semiconductor bulk materials are being explored to engineer these undesirable Schottky barriers. We present a theoretical study on the electron transport through metal-molecule-semiconductor interfaces. We use the B3PW91/LANL2DZ level of theory as implemented in the program Gaussian 03 to study a single molecule (2'-nitro-4-ethynylphenyl-4'-ethynylphenyl-benzen, named hereafter as mononitro) with a finite number (between 1 and 4) of Au and Si atoms attached at each end. Figure 1 shows an scheme of the systems when only one Au and one Si atom is attached to each end, for its neutral (left) , anion (center), and dianion (right) configurations. The same level of theory is used to study the bulk Si and Au using the program Crystal 03. Results from these two ab initio programs are used in our combined density functional theory-Green function (DFT/GF) approach (1) to calculate the DOS, transmission function, and current-voltage characteristics for these metal-molecule-semiconductor junctions. In order to account for the effect of the applied voltage in the molecule, the structure of the molecule are re-calculated for each value of the external bias electric field.

Figure 1. Mononitro systems attached to bulk Au and Si: neutral (left), anion (center), and dianion (right). Au (green), C (gray), H (white), N (blue), O (light blue), and Si (orange).

(1) Derosa, P. A.; Seminario, J. M. J Phys Chem B 2001, 105, 471-481.