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Transport Properties for Biphenyl-Based Molecular Junction System HISASHI KONDO, Institute of Industrial Science, University of Tokyo, JUN NARA, TAKAHISA OHNO, Computational Materials Science Center, National Institute for Materials Science — In the present study, the transport properties of an biphenyl-based molecule [X-BP-X (X: the end-group atom),X=O, S, Se, and Te] sandwiched between Au(111) electrodes are theoretically investigated using the non-equilibrium Green's function method based on the density functional theory. The end-group atom X has an influence on the interaction between the molecule and electrodes and the interaction between the two phenyl rings. For X =S, Se, and Te, similar transport properties are obtained, while the system with X =O exhibits much different properties from the other Xs. In case of X =O, the interaction between the molecule and electrodes becomes the weakest and that between π-type orbitals of the two phenyl rings, which mainly contributes to the transmission around the Fermi energy, becomes the strongest. As a result, this system has a larger transmission around the Fermi energy. We also investigate the dependence on dihedral angle between the two phenyl rings for all Xs. This study was supported by the RISS project and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government. The present calculations were performed by using the Numerical Materials Simulator in National Institute for Materials Science.

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