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Atomic-scale motor driven by the current-induced forces YU-CHANG CHEN, BAILEY C. HSU, ALLEN TSENG, Department of Electrophysics, National Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan —
From first-principles approaches, we investigate the current-induced forces in an asymmetric molecular junction using Hellmann-Feynman type theorem in the framework of density functional theory in scattering approaches. We observe that it is possible to construct atomic-scale systems where the current-induced forces can be used to rotate the atoms. As an example, we consider a junction formed by the benzene molecule which directly connected to the Pt electrodes, where the benzene molecule is highly tilted. The highly tilted benzene molecule causes the streamline flow of the current to curve considerably to one side of the benzene ring. This could cause a net torque due to the unbalanced current-induced forces, which tend to rotate the benzene molecule in a manner similar to a stream of water rotates a waterwheel. Thus, the highly asymmetric single molecule junctions offer the atomic-scale systems to explore the possibility of nano-motors driven by non-equilibrium electron transport. The authors thank National Science Council (Taiwan) for support under Grant NSC 100-2112-M-012-MY3

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