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**Dynamic Response to On/Off Signals in Nano Junctions** ZHANYU NING, McGill University, YU ZHU, JOSEPH MACIEJKO, JIAN WANG, HONG GUO, HONG GUO TEAM, JIAN WANG TEAM — We report the implementation of the time-dependent nonequilibrium Keldysh Green's function theorem (TD-NEGF). It provides a promising way to study the transient transport dynamics in nano devices by first principles calculation. Very importantly, we derive an efficient technique to overcome the singularity problem in the integration of spectrum function. The reliability of this method is carefully checked by a one-dimension chain model with the analytical solution. We then perform the ab-initio calculation in a realistic molecular junction (Al-Benzene-Al). The current dynamic response arises after applying an “upward” or “downward” step pulse, which predicts a characteristic timescale in transport dynamics of nano systems.

Zhanyu Ning  
McGill University

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