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The role of dimensionality on the molecule-lead coupling in molecular electronic junctions TAMAR ZELOVICH, Tel Aviv University, LEEOR KRONIK, Weizmann Institute of Science, ODED HOD, Tel Aviv University
— We present new insights into the role dimensionality plays in the lead-molecule coupling scheme at molecular electronic junctions. A key ingredient of our approach is a transformation of the Hamiltonian matrix from an atomistic to a state representation of the molecular junction. This provides direct access to the different couplings between the molecular states and the energy manifold of the leads, which underlie the transport properties of molecular junctions. We explore several tight-binding junction models and predict the appearance of coupling bands that depend on the dimensionality and shape of the leads. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

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