MODELING MOLECULAR JUNCTIONS: PITFALLS AND CAVEATS IN UNDERSTANDING QUANTUM TRANSPORT MECHANISMS AT THE MOLECULAR SCALE

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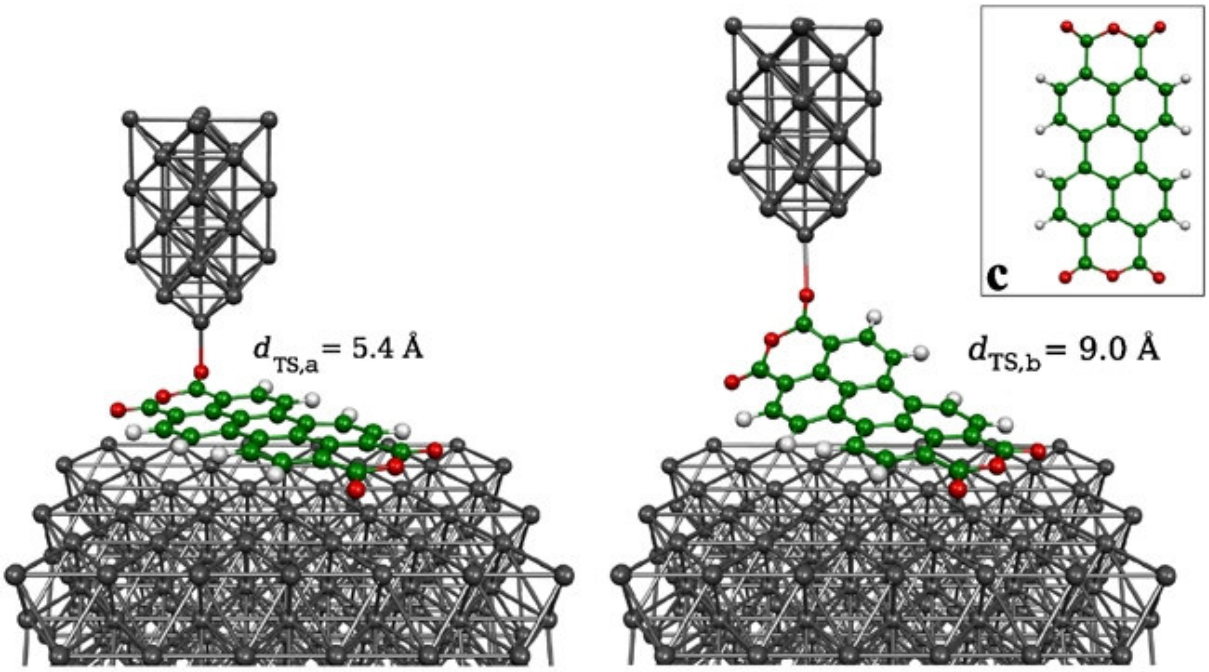
Since few years, several quantum transport experiments employing unimolecular systems have been proven. Some of related emerging phenomena, however, are still missing sound theoretical explanations. Principal limitations include the nature of the molecule-to-electrode contacts as well as the commonly used `static' and single particle description of molecular bridges. Molecules, indeed, are correlated flexible objects and indeed their 'mechanical' degrees of freedom play in general a fundamental role in charge transfer as well as transport mechanisms. In this talk, I will give an overview on the role of contacts, charging, vibrations and inelastic transport in molecular systems, and show how such phenomena do dramatically affect the overall conduction properties of STM-based molecular junctions.



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