

Abstract Submitted  
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**Theoretical Studies of Charge Transport through Al atomic wires** KHORGOLKHUU ODBADRAKH, PAWEL POMORSKI, CHRISTOPHER ROLAND, North Carolina State University — We have revisited the question of quantum transport through single-chain atomic Al wires, using a recently combined nonequilibrium/density functional-based formalism. Investigations of transport under a bias voltage brings additional insight into the current-voltage characteristics of this simple molecular electronic system. In agreement with previous work, we find that the Al-wires with (100) and (111) Al leads display prominent conductance oscillations with a period of four, that are qualitatively independent of lead size and configurations. A band structure analysis of the infinite Al-wire shows that this period may be explained in terms of induced resonance states localized at the atomic wire. In addition, we have investigated the induced charges in the wires as a function of the bias voltage, and the capacitance coefficients of the leads.

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