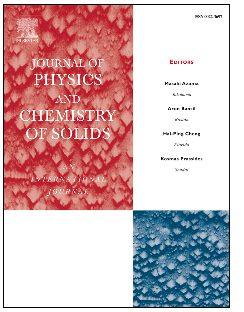

Influence of a thermal bath on the transport properties of an open molecular junction

Amir Eskandari-asl

PII: S0022-3697(18)30540-7

DOI: 10.1016/j.jpcs.2018.06.019

Reference: PCS 8633

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 5 March 2018

Revised Date: 2 June 2018

Accepted Date: 13 June 2018

Influence of a Thermal Bath on The Transport Properties of an Open Molecular Junction

Amir Eskandari-asl[a,1,]

[a]Department of physics, Shahid Beheshti University, G. C. Evin, Tehran 1983963113, Iran

Abstract

In a molecular junction (MJ) which connects two electrical leads, electron-phonon coupling has significant effects on the transport properties. However, the MJ is not thermally isolated and the phonons can be coupled to another thermal bath. For strong enough couplings, the bath thermalizes phonons on the MJ so that their number would be bias independent. However, in medium and weak coupling regimes, the number of phonons created in MJ depends on the bias voltage. Obtaining the master equation (ME) for this system and comparing the results with the case where we have no such thermal bath, we show that if the bath temperature is greater than the leads, at low bias voltages (where in the absence of the thermal bath the probability of phonon excitation is low), the thermal bath heats up our MJ and decreases electronic current. On the other hand, at high bias voltages the bath cools down MJ and increases the current. However, if the bath temperature is less than the leads, it always increases the current and the heat flows from the junction to the leads.

Keywords: electron-phonon coupling, heat flow, Frank-Condon blockade, effective temperature

1. Introduction

Recent advances in nanotechnology paves the way into molecular electronics, with MJ as an important building block[1, 2]. MJs which are molecular sized quantum dots (QDs) that connect electrical leads, have been the subject of many experimental and theoretical studies [3, 4, 5, 6, 7, 8, 9].

One main difference between large QDs and MJs is that in the latter there exist a noticeable electron-phonon coupling. This coupling substantially affects transport properties of the system and may result in phenomena such as Frank-Condon blockade, negative differential resistance, etc[10, 11, 12].

One theoretical approach is to trace out the leads degrees of freedom and obtain a ME which describes the dynamics of MJ (electrons and phonons)[9,

Email address: a_eskandariasl@sbu.ac.ir; amir.eskandari.asl@gmail.com (Amir Eskandari-asl)