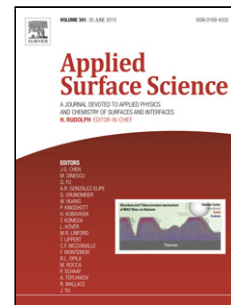


## Accepted Manuscript

Title: The effect of electrodes on 11 acene molecular spin valve: Semi-empirical study

Authors: A. Aadhityan, C. Preferencial Kala, D. John Thiruvadiga



PII: S0169-4332(17)30548-2  
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.02.175>  
Reference: APSUSC 35284

To appear in: *APSUSC*

Received date: 15-10-2016  
Revised date: 14-2-2017  
Accepted date: 19-2-2017

Please cite this article as: A.Aadhityan, C.Preferencial Kala, D.John Thiruvadiga, The effect of electrodes on 11 acene molecular spin valve: Semi-empirical study, Applied Surface Science <http://dx.doi.org/10.1016/j.apsusc.2017.02.175>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## The effect of electrodes on 11 acene molecular spin valve: Semi-empirical study

Aadhityan A<sup>1</sup>, Preferencial Kala C<sup>1\*</sup> [preferencialkala.c@ktr.srmuniv.ac.in](mailto:preferencialkala.c@ktr.srmuniv.ac.in), John Thiruvadigal D<sup>1</sup>

<sup>1</sup>Department of Physics and Nano Technology, Center for Materials Science and Nanodevices, SRM University, Kattankulathur - 603 203. India.

\*Corresponding author: Dr. Mobile number: +91-9791034080, Fax: +91-44-27453903,

### Highlights

- A semi-empirical approach to analyze the electron transport characteristics of 11 acene molecular spin valve
- the effect of electrodes modifying the spin-dependence behaviours of these systems in a controlled way
- Iron electrode is an efficient one to construct 11-acene single molecular spin valve

### Abstract

A new revolution in electronics is molecular spintronics, with the contemporary evolution of the two novel disciplines of spintronics and molecular electronics. The key point is the creation of molecular spin valve which consists of a diamagnetic molecule in between two magnetic leads. In this paper, non-equilibrium Green's function (NEGF) combined with Extended Huckel Theory (EHT); a semi-empirical approach is used to analyse the electron transport characteristics of 11 acene molecular spin valve. We examine the spin-dependence transport on 11 acene molecular junction with various semi-infinite electrodes as Iron, Cobalt and Nickel. To analyse the spin-dependence transport properties the left and right electrodes are joined to the central region in parallel and anti-parallel configurations. We computed spin polarised device density of states, projected device density of states of carbon and the electrode element, and transmission of these devices. The results demonstrate that the effect of electrodes modifying the spin-dependence behaviours of these systems in a controlled way. In Parallel and anti-parallel configuration the separation of spin up and spin down is larger in the case of iron electrode than nickel and cobalt electrodes. It shows that iron is the best electrode for 11 acene spin valve device. Our theoretical results are reasonably impressive and trigger our motivation for comprehending the transport properties of these molecular-sized contacts.

**Keywords** : Nonequilibrium green's function, Density functional theory, Spin-dependence transport, molecular spin valve

Download English Version:

<https://daneshyari.com/en/article/5350166>

Download Persian Version:

<https://daneshyari.com/article/5350166>

[Daneshyari.com](https://daneshyari.com)