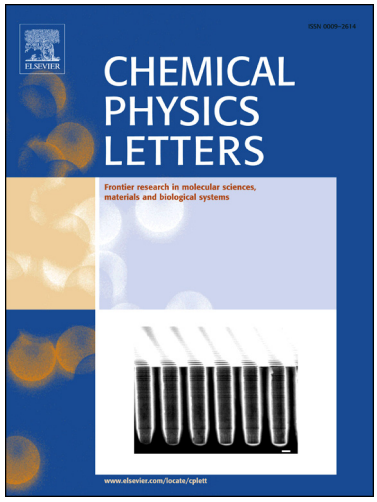

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First principles study of mixed-stack charge transfer pyromellitic diimide - diamino pyrene (PMDI - DAP) derivative

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Abstract

Room temperature ferroelectric based on PMDI-DAP co-crystal (Tayi et al. *Nature* **2012**, *488*, 485–489) was extensively investigated by means of *abinitio* DFT methodology. The study constitute geometry optimisation, band structure calculations and potential energy surface scan of modelled polarisation switching path of the mixed stack. Further, quantum chemical calculations of the charge-transport parameters of isolated molecular clusters are performed to rationalize the band structure results. We also comment on the viability of integrating the organic ferroelectric into non-volatile memory device in the light of calculated results.

Keywords: Organic Ferroelectric, Charge Transfer Complex, DFT, Non-volatile Memory

1. Introduction

Ferroelectrics are important functional materials of both fundamental and technological interest. Ferroelectrics find application in numerous present day technologies ranging across Random Access Memory (FeRAM), Field-effect transistors (FeFET), transducers, electron emitters, non-linear optical devices, infrared detectors, piezoelectric sensors etc.[1, 2]. Traditionally, inorganic materials such as $BaTiO_3$, Pb$(Zr_xTi_{1-x})O_3$ or hybrid inorganic-organics like triglycine sulfate(TGS) holds major share in ferroelectric do-

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