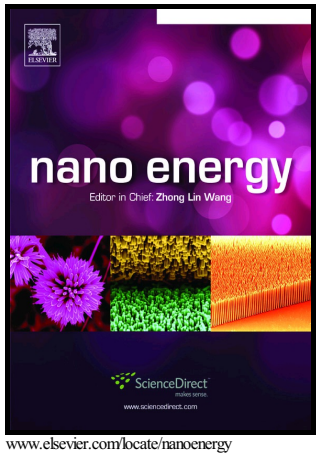

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PII: S2211-2855(16)30191-4
DOI: http://dx.doi.org/10.1016/j.nanoen.2016.06.011
Reference: NANOEN1329

To appear in: *Nano Energy*

Received date: 23 January 2016
Revised date: 30 May 2016
Accepted date: 7 June 2016

Cite this article as: Supratik Kar, Natalia Sizochenko, Lucky Ahmed, Victor S Batista and Jerzy Leszczynski, Quantitative Structure-Property Relationshi Model Leading to Virtual Screening of Fullerene Derivatives: Exploring Structural Attributes Critical for Photoconversion Efficiency of Polymer Sola Cell Acceptors, *Nano Energy,* http://dx.doi.org/10.1016/j.nanoen.2016.06.011

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Abstract:

The power conversion efficiency (PCE) of pure polymer solar cells (PSCs) remains low, although significantly higher values could be achieved by using PSCs as carrier donors in conjunction with composite fullerene derivative (FD) acceptors. Significant resources, however, are required to experimentally develop and screen FDs that may serve as efficient acceptors in PSCs. Often, the materials are expensive, the methods are time consuming, and the production processes can generate toxic hazards. As an alternative approach, we introduce a quantitative structure-property relationship (QSPR) model for predicting the PCE of 59 FDs, including both C_{60} and C_{70} FDs. The QSPR model enables identification of the essential structural attributes necessary for quantifying the molecular prerequisites of diverse FDs, chiefly responsible for high PCE of PSC acceptors in composition with poly(3-hexylthiophene) (P3HT). The identified properties and structural fragments are particularly valuable for guiding future synthetic efforts for development of FDs with improved power conversion efficiency. Furthermore, a large number of FDs are collected to generate a database. Virtual screening of the database employing the developed QSPR model allows for identification of nine FDs with higher PCE than previously studied FDs.

Graphical abstract