Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Data Mining with Molecular Design Rules Identifies New Class of Dyes for Dye-Sensitized Solar Cells JACQUELINE COLE, University of Cambridge, UK & Argonne National Laboratory, USA — A major deficit in suitable dyes is stiffling progress in the dye-sensitized solar cell (DSC) industry. Materials discovery strategies have afforded numerous new dyes; yet, corresponding solution-based DSC device performance has little improved upon 11% efficiency, achieved using the N719 dye over two decades ago. Research on these dyes has nevertheless revealed relationships between the molecular structure of dyes and their associated DSC efficiency. Here, we have codified such structure-property relationships in the form of molecular dye design rules, which have been judiciously sequenced in an algorithm to enable large-scale data mining of dye structures with optimal DSC performance. For the first time, we have a DSC-specific dye-discovery strategy that predicts new classes of dyes from surveying a representative set of chemical space. A lead material from these predictions is experimentally validated herein, showing DSC efficiency that is comparable to many well-known organic dyes. This demonstrates the power of this approach.

Jacqueline Cole
University of Cambridge, UK & Argonne National Laboratory, USA

Date submitted: 15 Nov 2013 Electronic form version 1.4