Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A framework for the design of nanomaterials with targeted applications[1] VLADAN MLINAR, School of Engineering, Brown University, Providence, RI 02912, USA — Engineered nanomaterials are the key building blocks of modern optoelectronic devices and understanding their structure-property relationship can lead to breakthroughs in device design. Even if we suspect that there may be many structures that are consistent with the targeted property, finding a single one may be a daunting, but often also unnecessary, task because of the enormous space of material parameters. Here, I will show how to parametrize the structure via a set of structural features using the targeted physical property as a constraint. Structural features are extracted from our procedure such that they are relevant to the targeted property/ies and linked to the underlying full atomistic structure. I will discuss the conditions under which the representation of the structure via structural features can be very similar, ideally equivalent, to the full structure *only* relative to our targeted properties. Finally, I will demonstrate the importance and validity of the approach using the example application of engineered nanomaterials for third-generation photovoltaics solar cells.

[1]Supported by Brown University Faculty Development Fund and NASA EPSCoR.

Vladan Mlinar
School of Engineering, Brown University, USA

Date submitted: 08 Nov 2012 Electronic form version 1.4