A framework for the design of nanomaterials with targeted applications

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.

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