n::CAD a novel suit for nanotecnology

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Abstract

n:: CAD is conceived as a new tool for the design, modeling and simulation of the physical properties of systems and devices at the nanoscale. The main aim of the software platform is to build a productive environment for a sequential and concurrent multiscaling analysis, connecting the design capabilities of traditional computer aided design software (CAD) at the macroscale and the atomistic representation of matter, as well as provide an intensive use of computational atomistic methods that have been developed by the scientific community to calculate physical properties at the atomic scale. The platform includes a complete atomic editor for molecules, bulk and 0/1/2/3 D materials, that permits the incorporation of almost any type of defects, and it also enables the atomic building and the orientation matching of systems and devices built by CAD or in-platform tools. It also includes a library of materials for a preconfigured analysis, a powerful atomic visualizer for any kind of systems, including atomic representation of real size ensembles, and post-processing tools. Proprietary, third-party and open-source codes from different methodologies and theoretical frameworks are connected through modules that permit the specific generation of input files and an in-platform post-processing. All this features are integrated in a friendly, dynamic, intuitive and innovative graphical user interface that enables an easy use of sophisticated modeling and simulation tools, usually difficult to use, to experts from different worlds. We are open and happy to include and work with new methods that would enrich the n:: CAD platform.

References

n/a.

Figures

Illustration of scaling

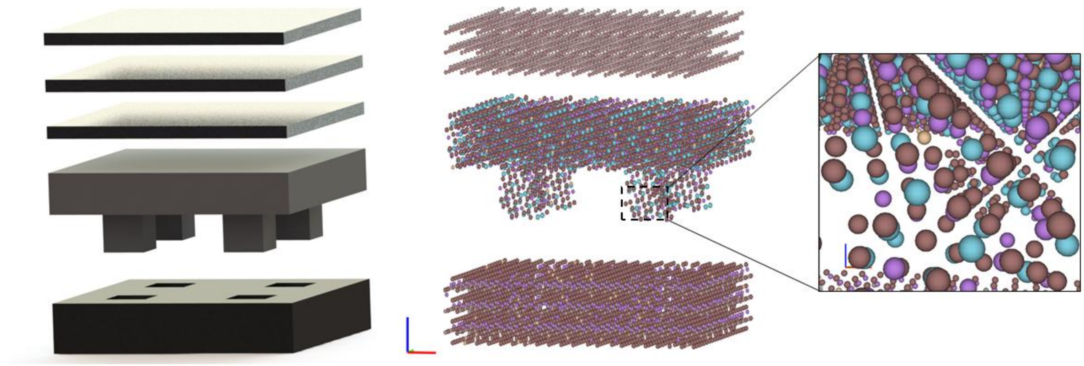

Illustration of defects modeling