

n::CAD, bringing together the macro & continuous world with the atomic description at the nanoscale

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Abstract: nCAD is an innovative software that connects 3D-CAD design programs and atomic visualization. nCAD provides a friendly and common environment for modelling, visualization and post-processing in the atomic scale with a powerful graphical user interface (GUI). nCAD permits to build the atomic structure of an assembly designed by a CAD software (SolidWorks), furthermore simple 3D pieces can be built inside the GUI and combined with the CAD models. The unit cells for the different components can be created in the GUI or imported from internal libraries and external sources. nCAD understands symmetry and allows for surface cells. Another innovative feature is the possibility of implementing point and pair defects distributed throughout the material (occupation, interstitials, substitutionals, Frenkel, Schottky, etc.). nCAD allows to set the crystallographic orientation and to adjust it with the spatial orientation and the real shape of the 3D models. nCAD includes an automatic generator of nanotubes and low dimensional structures.

The visualizer includes a big number of graphical tools and full control of the objects in the scene. Different visualizers have been implemented in order to work with the unit cell, the atomic structure of a real 3D piece or with an assembly. All the visualizers offer dynamical and "on the fly" information of the system to the user.

nCAD permits the post-processing of the results of atomic simulations in the same platform and with a simultaneous visualization of the inputs and results. nCAD is able to create isosurfaces, isolines, several schemas of colour maps and to project the results over planes and specific geometries.

nCad is now compatible with SimPhoNy, a multi-scale modeling environment for nano-materials and system design, and nFLUID, also develop by Sgenia.

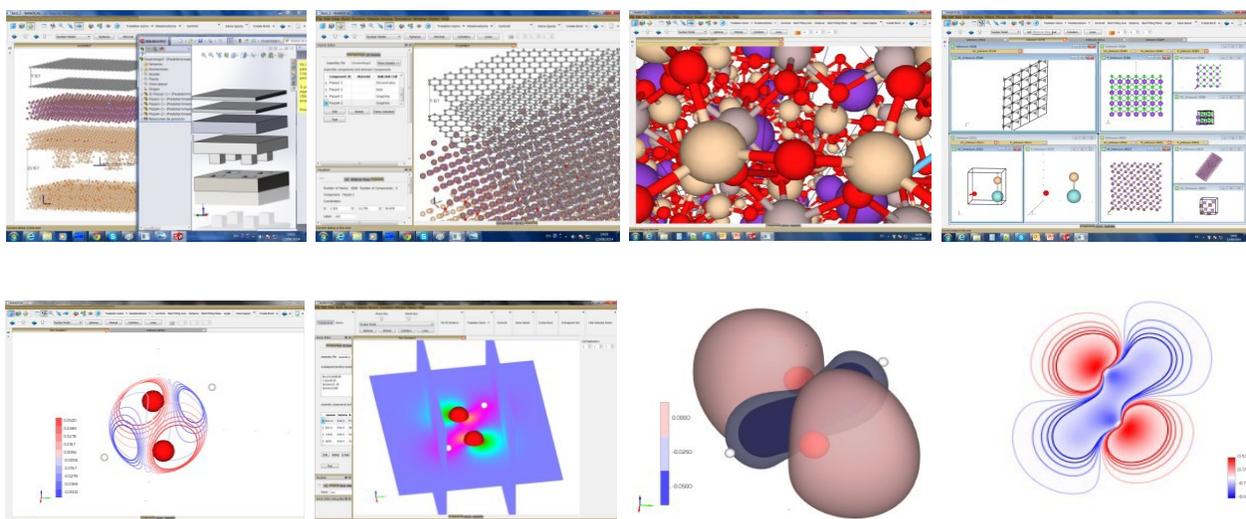


Figure 1: Eight snapshots illustrating different features of nCAD.