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Generalizing the Quantum Dot Lab Towards Arbitrary Shapes and Compositions

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ABSTRACT

As applications in nanotechnology reach the scale of countable atoms, computer simulation has become a necessity in the understanding of new devices, such as quantum dots. To understand the various optoelectronic properties of these nanoparticles, the Quantum Dot Lab (QDL) has been created and powered by NEMO5 to simulate on multi-scale, multi-physics bases. QDL is easy to use by offering choices of different QD geometries such as shapes and sizes to the users from a predefined menu. The simplicity of use, however, limits the simulation of general QD shapes and compositions. A method to import generic strained crystalline and amorphous dot structures into the QDL has been created here. Users can now analyze electronic structure effects in both effective mass and 10-band sp3d5s* tight-binding models. Implementation has been successful through a restructuring of the user interface as well as the alteration of the primary bodies of Tcl code that interpret input and pass them on to NEMO5 for precision computation. With this new development comes the ability for researchers, educators, and students alike to peer into uncharted areas of quantum technology and gain new insight through a high-level of simulation plasticity.

KEYWORDS

Quantum dots, generic structure, strained crystalline, amorphous