



Virtual Synthesis of Nanosystems by Design: From First Principles to Applications (Elsevier Insights)

Liudmila Pozhar

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This is the only book on a novel fundamental method that uses quantum many body theoretical approach to synthesis of nanomaterials by design. This approach allows the first-principle prediction of transport properties of strongly spatially non-uniform systems, such as small QDs and molecules, where currently used DFT-based methods either fail, or have to use empirical parameters. The book discusses modified algorithms that allow mimicking experimental synthesis of novel nanomaterials---to compare the results with the theoretical predictions--and provides already developed electronic templates of sub-nanoscale systems and molecules that can be used as components of larger materials/fluidic systems.

- The only publication on quantum many body theoretical approach to synthesis of nano- and sub-nanoscale systems by design.
- Novel and existing many-body field theoretical, computational methods are developed and used to realize the theoretical predictions for materials for IR sensors, light sources, information storage and processing, electronics, light harvesting, etc. Novel algorithms for EMD and NEMD molecular simulations of the materials' synthesis processes and charge-spin transport in synthesized systems are developed and described.
- Includes the first ever models of Ni-O quantum wires supported by existing experimental data.
- All-inclusive analysis of existing experimental data versus the obtained theoretical predictions and nanomaterials templates.

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