Compuational NanoMaterials Design: From Basics to Actual Applications

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We entered the 21st Century witnessing several remarkable progress in Science and Technology. Novel materials and devices that were once considered *science fiction* materials are, one after the other, becoming a reality. On the other hand, as is always the case, progress comes at a price. In the process of furthering progress in Science and Technology, we encounter new problems and agenda where conventional techniques and routines no longer apply. A case in point is the astonishing development seen in nanometer scale technology, Nanotechnology. To meet the ever-increasing demand for better large scale integration, basic components of devices are getting smaller and smaller, with the size ranging from the nanometer-scale to atomic sizes. One can easily realize that *Quantum Effects* would become increasingly important. (As to how they will be important is something we are in the stage of discovering.) However, we would not be exaggerating too much if we say that with further development, there will come a time when the basic material entity that is used to build a device, would, by itself, be made to function as a device. Given these circumstances, there is an ever-increasing demand to develop novel theoretical routines and techniques that could quickly and efficiently find novel materials for synthesis, that would suit our purposes. The theoretical routines and techniques necessary should incorporate quantum mechanics per se, and should not be dependent on experimental results and/or empirical parameters. *Ab-Initio/First Principles Calculations* satisfy all these requirements. It should be noted that the ab-initio/first principles calculation we are mentioning here are based on the *Density Functional Theory*, which follows naturally from the basic principles of quantum mechanics. With recent developments in computational techniques, coupled with the rapid progress in computer efficiency, ab-initio/first principles-based *COMPUTATIONAL MATERIALS DESIGN* (**CMD**®) [1, 2] is now a reality. Its impact/influence on industrial R&D should increase with the passing years. It is worth mentioning that there are already several precedents of patents granted for application based purely on the application of CMD® techniques, and more are expected to follow. At the meeting, we will briefly introduce the basic foundations/principles of CMD® and the actual novel materials, e.g., benzene-transition metal multiple-decker sandwich cluster and chain that were realized experimentally [3-4] and investigated using CMD® techniques [5-7].

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