

## Mathematical formalisms of small structures of materials, properties and Technologies



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In general, materials when made self-confined in a pretty small size render surface controlled tunable structures, energy carriers, properties and in turn exotic applications. Surface species become mobile like a rheological fluid self-confined in a small space  $0 \rightarrow 2D$  of the material. So, such materials behave differently in thermodynamics than the counterpart bulk materials. As a result, traditionally, these are so called ‘smart nanomaterials’, wherein the energized surface atoms contain (i) lower co-ordination number, (ii) lower atomic density, (iii) lower symmetry, (iv) larger interatomic distance, and (v) larger entropy/enthalpy in a high-energy state over the thermodynamic equilibrium state of its bulk structure. Mathematically, these are five basic exotic stimuli that determine, control, and monitor tailored high-energy thermodynamic stability, structure, energy-carriers, profound properties and applications of a given material over those in its bulk state in a correlation of structure–properties–technology. As a result, altogether this is a new class of ‘synergistic materials’, with tunable distributions of density of states of electrons or other energy-carriers, which promptly control the properties. Some of these basic points will be addressed in this invited talk with selected examples of different kinds of formalisms of functional materials (especially, those of duly small sizes, which deliver size dependent tunable properties for multiple applications), their innovative crystal structures and engineered properties for selective energy, photocatalysis, photonics, spintronics, and other applications in science, technology, medicines, foods, and other fields in integral parts on our day-to-day growing demands and utilities. As usual, such materials neither truly obey the well-known laws of quantum mechanics nor that of the classical mechanics either. In fact, it is a “hierarchical cluster” of multiple energy-carriers that promptly governs the exotic properties and applications.

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