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Quantum Boundary Effect on Electronic Structures of Nanomaterials Y.Y. SUN, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, KYUHO LEE, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, D. WEST, S.B. ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, RENSSELAER POLYTECHNIC INSTITUTE TEAM, RUTGERS UNIVERSITY TEAM — Nanosciences are, to a large extent, related to the quantum size effect. Nanomaterials with similar characteristic sizes, however, do not necessarily exhibit similar quantum effects, e.g., the shape of the nanomaterials is known to affect their electronic properties also. Other than the size and shape, the boundary of a nanostructure, from which the quantum confinement arises, is another key factor that affects the expressions of the quantum effects. Here, we discuss a quantum boundary effect on the electronic structures of nanomaterials. We argue that different boundary atomic structures of nanomaterials of the same characteristic size and shape could be energetically degenerate, but give distinct electronic properties, e.g., band gaps. Such an effect could pose a challenge on preparing nanomaterials with expected electronic properties. Our discussion will be based on first-principles electronic structure calculations.

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