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Electronic Structure of Bimetallic Core/Shell Quantum-Dots RUBEN ESTRADA-SALAS, HECTOR BARRON, DEVRAJ SANDHU, MIGUEL JOSE-YACAMAN, University of Texas at San Antonio — A quantum-dot (QD) is a nanoscale structure consisting of one or more semiconducting materials in which the motion of fundamental charge carriers is confined in all spatial dimensions. Core/shell quantum-dots (CSQDs) are a variety of QD consisting of two sections: An ellipsoidal core is manufactured from one material, and a shell of a second material is added around this. QDs have been the subject of great scientific and technological interest, with promising applications that include display devices, biological tagging materials, photovoltaics, and lasers. In this work, the electronic structure of bimetallic CSQDs (size < 2 nm) is analyzed by using Density-Functional Theory (DFT), with the end of correlate their electronic properties with their potential applications. We select the Au/Ag, Au/Pd and Au/Pt systems because of the experimental studies reported on these systems.

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