How Do We Simulate the Next Generation of Materials? From Newton to Schrödinger's Cat: HPC, AI and Quantum Computing

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Simulating the next generation of materials will require the convergence of physics-based modeling, high-performance computing (HPC), artificial intelligence (AI), and emerging quantum-computing paradigms. This lecture presents a journey across this evolving computational landscape and the tools that future researchers will need to master.

We begin with classical molecular dynamics and LAMMPS, connecting Newton's equations of motion with atomistic trajectories and measurable properties [1]. We then move to density functional theory (DFT), where an explicit quantum-mechanical description becomes necessary to understand chemical bonding, electronic structure, and catalytic activity, illustrated with supported Au clusters [2].

The central case study is our recent investigation of a new family of hollow Au60 nanocages [3]. Their structural topology, energetics, and finite-temperature stability reveal a counterintuitive result: high symmetry does not necessarily imply high stability. Instead, local coordination and connectivity emerge as key factors, illustrating how electronic-structure calculations, atomistic simulation, HPC, and machine-learning approaches can converge within a single computational workflow.

From finite nanostructures, we move toward 2D and 2.5D van der Waals heterostructures and moiré quantum materials, where strong correlations, Mott-like states, topology, and superconductivity pose new computational challenges.

These examples motivate the central question: how do we simulate materials whose configurational and quantum complexity exceeds any single computational paradigm? HPC, AI, and Quantum Computing should therefore be viewed not as competing technologies, but as complementary tools. For the next generation of scientists, the challenge is not simply to master a code, but to understand the physics well enough to choose, combine, question, and validate computational methods across scales — from Newton's equations to Schrödinger's quantum world.

1. In-Situ TEM Study of Mechanical Behavior of Twinned Nanoparticles, G. Casillas-García, J.P. Palomares-Báez, J.L. Rodríguez-López, J. Luo, A. Ponce, R. Esparza, J.J. Velázquez-Salazar, A. Hurtado-Matías, and M. José-Yacamán. Philosophical Magazine 92, 4437 (2012). https://doi.org/10.1080/14786435.2012.709951 .

2. Experimental and DFT Studies of Gold Nanoparticles Supported on MgO(111) Nano-sheets and Their Catalytic Activity. Z. Li, C.V. Ciobanu, J.P. Palomares-Báez, J.L. Rodríguez-López, and R. Richards. Phys. Chem. Chem. Phys. 13, 2582 (2011). https://doi.org/10.1039/C0CP01820A .
3. A new family of hollow Au60 cages: topological diversity and connectivity-driven stability. E.E. Hernández Vázquez, R.H. Aguilera del Toro, J.M. Nápoles Duarte, J.M. Montejano Carrizales, F. Aguilera Granja, I.L. Garzón, J.L. Rodríguez López, J.P. Palomares Báez. Nanoscale 18, 1673 (2026). https://doi.org/10.1039/d6nr01764a .

José Luis Rodríguez López a theoretical physicist trained at the Autonomous University of San Luis Potosí, he completed a postdoctoral fellowship at the Texas Materials Institute at the University of Texas at Austin.

A common thread throughout his 35 years of scientific training and research career has been the relationship between structure and function in materials: how controlling size, shape, composition, connectivity, and interfaces at the nanoscale makes it possible to modify properties and advance toward the rational design of materials and applications—shape determines function; properties and applications by design.

This vision has been consolidated through his research areas: **Nano in silico**, devoted to the computational modeling and design of nanostructures; **Nano for Environmental Remediation**, with an emphasis on photocatalysis and hydrogen generation; **Nano for Health**, focused on the design and functionalization of nanoparticles for nanomedicine; **Nano for Education**, dedicated to teaching, science outreach, and the development of STEM vocations; and, more recently, **2D and 2.5D van der Waals Materials**, which extends these principles to graphene, two-dimensional materials, and their heterostructures for new scientific and technological applications.

He is currently a Professor of Physics at the National Autonomous University of Mexico (UNAM), and is a member of Mexico's National System of Researchers (Sistema Nacional de Investigadoras e Investigadores). He combines fundamental research with R&D&I activities in advanced materials, building bridges between fundamental science, materials design, and technological applications in industry.