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Future directions in the simulation of nanomaterials

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Nanotechnology forces us to rethink conventional solid state physics. Quantum phenomena are commonplace. A system with 101 atoms may be very different from one with just 100. Key biomolecules may resemble spaghetti more than silicon; viscosity often dominates over inertia. Statistical physics is often not carrier statistics; equilibrium may be irrelevant, though the kinetics of non-equilibrium processes can be crucial. Even when nanoscale issues concern structure (rather than functionality), a new viewpoint is needed. Important features, like elasticity and electrostatic energies, have clear macroscopic analogies, but different issues arise, reflecting the reproducibility of quantum dots or the accuracy of self-organisation. Concepts like epitaxy and templating are usually micro- or meso-structural, but emerge again in modelling for the nanoscale. Unexpected analogies between biomolecule and semiconductor systems appear. My examples will include quantum dots and possible silicon-based, room temperature, quantum information processing, and will emphasise new opportunities in nanoscale science.