

Physics Colloquium
Friday, 6 November, 4:10 P.M.

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Quantum Electrostatics at the Atomic Scale

Physics Room 130

social half-hour starting 3:40 P.M.

Over the years, physicists have developed methods for calculating the properties of materials from first principles (that is, by solving the Schrödinger equation for the electrons) in situations of increasing complexity. Today it is possible to compute the nonlinear capacitance of an ultrathin capacitor composed, say, of four unit cells of BaTiO_3 sandwiched between platinum electrodes. I will discuss some of the challenges that have had to be overcome to arrive at such a capability, including the development of methods for computing electric polarization (one cannot just sum dipoles!) and for treating insulators in a finite electric field (even though there is no ground state!). Then I will show how some of the concepts of elementary electrostatics, such as the usefulness of the electric displacement field \mathbf{D} , can be extended all the way down to the atomic level. For an application, I will present calculations of the minimum thickness for ferroelectricity in ultrathin ferroelectric capacitors, showing that in some cases there is no minimum thickness at all.

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