relation at all, thereby reducing the complexity of the calculation by as much as 90%. Technically, any process that considers electrons two at a time must scale at least like N^2. But the prescreening was a small enough part of the whole calculation that the overall method scales almost like N.

Earlier this year Riplinger and Neese presented their nearly linear method for CCSD,[2] which they've dubbed "domain-based local PNO-CCSD." And now they and their colleagues have applied the same methods to the perturbative triples correction, resulting in DLPNO-CCSD(T).[3]

Large molecules

Even with all the approximations and truncations made by DLPNO-CCSD(T), the researchers found that it still captures more than 99.8% of the standard CCSD(T) correlation energy for a test set of medium-sized organic molecules. And they were able to calculate coupled-cluster energies for far larger molecules than had ever been possible before, including the linear hydrocarbon $C_{150}H_{302}$ and the 644-atom protein crambin, shown in figure 2. "I was remembering that a few years back, Filipp Furche and John Perdew presented a calculation on the crambin molecule using RI-DFT," says Neese, referring to resolution of the identity density-functional theory, the most efficient DFT method.[7] "That was a spectacular calculation in 2006." By working with the three-dimensional electron density rather than the $3N$-dimensional N-electron wavefunction, DFT has a natural efficiency advantage over wavefunction methods, so it's often the approach of choice for studying large molecules. But its accuracy has yet to rival that of CCSD(T).

Neese and colleagues are continuing to work toward making their DLPNO-based coupled-cluster methods as useful as possible for users' calculations. For example, they hope to develop a code to treat molecules such as ozone, which aren't easily studied with coupled-cluster theory because they have unpaired electrons and aren't well approximated by a single reference state. They plan to make all their methods available to users via their software package ORCA. **Johanna Miller**

References

1. R. J. Bartlett, M. Musiał, *Rev. Mod. Phys.* **79**, 291 (2007).
2. C. Riplinger, F. Neese, *J. Chem. Phys.* **138**, 034106 (2013).
3. C. Riplinger et al., *J. Chem. Phys.* **139**, 134101 (2013).
4. F. Neese, F. Wennmohs, A. Hansen, *J. Chem. Phys.* **130**, 114108 (2009); F. Neese, A. Hansen, D. G. Liakos, *J. Chem. Phys.* **131**, 064103 (2009).
5. M. Schütz et al., *J. Chem. Phys.* **138**, 054109 (2013).
6. P. Pulay, *Chem. Phys. Lett.* **100**, 151 (1983).
7. F. Furche, J. P. Perdew, *J. Chem. Phys.* **124**, 044103 (2006).

physics update

These items, with supplementary material, first appeared at http://www.physicstoday.org.

How annoying is wind-turbine noise? As the harnessing of wind power as a renewable energy source has grown, so too has the debate over possible sleep loss and other physiological effects from the noise generated by wind turbines.

Primarily arising in aerodynamic boundary layers along the rotating turbine blades, the sounds are amplitude modulated, with a characteristic "swish" at a frequency of about 1 Hz. Periodic sounds are more readily perceived than constant noise sources (see, for example, PHYSICS TODAY, August 2013, page 19). Indeed, studies report that people are more likely to be annoyed by low levels of turbine noise than by much louder noise from transportation and other industrial sources. The degree of annoyance from turbine noise shows little correlation with the average sound level, termed the equivalent continuous sound-pressure level, yet that parameter is commonly used in noise regulations. To better understand the perception of turbine noise, Yeolwan Seong, Soogab Lee, and colleagues from Seoul National University have studied different ways of parameterizing the sounds. The researchers had test subjects in an anechoic chamber listen to simulations of wind-turbine noise at varying distances and orientations; for each sample, the subjects recorded their degree of annoyance on a seven-point scale. The team found that the listeners' responses were best explained statistically not by the average sound level or fluctuation level but by the maximum instantaneous sound level, a parameter frequently used in criteria regulating nighttime (and some daytime) intermittent noise sources. (Y. Seong et al., *J. Renewable Sustainable Energy* **5**, 052008, 2013.) —RJF

Taming topological defects with light. Real crystals are rarely perfect; they tend to contain the occasional defect, such as the one in the colloidal packing depicted here. The packing is visualized as a Voronoi diagram, with each 2-μm-diameter colloidal particle represented by a polygonal cell. In what's known as a dislocation, two extra rows of particles, indicated by dashed yellow lines, have been squeezed into the hexagonal lattice, leaving one particle (white) with only five nearest neighbors and another (gray) with seven. (For more on colloidal crystals, see PHYSICS TODAY, September 2010, page 30, and December 1998, page 24.) A form of topological defect, dislocations are common in both colloidal and atomic crystals. Understanding how they emerge and interact is key to modeling the kinetics of melting and of solid-to-solid phase transitions. But experimentalists have lacked the means to reproducibly control such defects in the lab. Now William Irvine (University of Chicago), Paul Chaikin (New York University), and their coworkers have demonstrated a way to manipulate colloidal-lattice dislocations using arrays of holographically generated optical traps. Dubbed topological tweezers, the arrays can capture dozens of particles simultaneously—each particle in its own potential well—such that clusters of particles can be pushed or pulled in unison. By strategically nudging selected clusters, the researchers can create, steer, and even induce fission of lattice dislocations. They can also rotate a cluster to create a grain boundary. But curiously, reversing the rotation doesn't return a pristine lattice; it only causes the boundary to expand. (W. T. M. Irvine et al., *Proc. Natl. Acad. Sci. USA* **110**, 15544, 2013.) —AGS