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A New Wave In Water Modeling

For decades, theorists have been wrestling with ways to model water's complicated behavior, such as its expansion when it freezes and its propensity for forming clusters. Now, Krzysztof Szalewicz at the University of Delaware and colleagues say they've developed a method that accurately describes water using only the basic principles of physics, without experimentally derived values for key parameters (Science 2007, 315, 1249). Adding experimental data to models can help chemists accurately predict some aspects of water but often at the expense of others. A purely ab initio, or first principles, model, however, would allow scientists to better explore exotica such as polymorphic forms of ice or supercritical phases. The researchers meshed several long-standing theoretical methods to create a function that predicts water's properties for the liquid (shown) and for the water dimer. Some scientists caution that more work is needed, especially in the realm of dynamics, whereas others say the work is an important step forward. "The authors have been able to show that a good description of water from first principles is becoming feasible," writes the University of Cambridge's Anthony J. Stone in an accompanying commentary.

Toward Ovarian Cancer Biomarkers

By the time doctors detect ovarian cancer in a patient, it's usually too late for successful treatment. More timely diagnosis could be one eventual payoff of efforts to identify early-stage biomarkers. Toward that end, a team of Swedish researchers led by Peter James at Lund University reports the results of a