Resolving the high pressure phases of calcium

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(PhysOrg.com) -- Significant experimental and theoretical work has been devoted to the electronic, structural and superconducting properties of calcium (Ca) at high pressure.

New research by Laboratory scientists resolves a controversy between theory and experiment about the finite and low-temperature stability of Ca at very high pressures (between 40,000 and 1.1 million atmospheres of pressure).

Ca has noteworthy superconducting properties. Starting at about 45,000 atmospheres of pressure, the superconducting critical temperature increases with pressure and reaches up to 25 Kelvins at 1.6 million atmospheres. However, the structure in which it becomes a superconductor is still being debated.

The Livermore team used a combination of density functional theory (DFT) and quantum Monte Carlo calculations (QMC) to get to the bottom of the disagreement. The team, made up of A. Teweldeberhan, Jonathan DuBois and Stanimir Bonev, showed that the standard exchange-correlation approximations used in DFT yield significantly inaccurate energies for dense Ca. Such calculations have been used in a large number of studies to predict the structures and other properties (notably superconductivity) of Ca.

"This finding will be of significant and broad interest," Bonev said. "It not only reports important results for Ca, but also has more general

implications for the use of DFT methods to study materials under extreme conditions, where electronic changes similar to that found in Ca are common."

The research appears in the Dec. issue of Physical Review Letters.

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