

Low-temperature phase of the Cd₂Re₂O₇ superconductor: ab initio phonon calculations and Raman scattering

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Using an *ab initio* approach, we report a phonon soft mode in the tetragonal structure described by the space group $I4_122$ of the 1 K 5d superconductor Cd₂Re₂O₇. It induces an orthorhombic distortion to a crystal structure described by the space group $F222$ which hosts the superconducting state. This new phase has a lower total energy than the other known crystal structures of Cd₂Re₂O₇. Comprehensive temperature dependent Raman scattering experiments on isotope enriched samples, ¹¹⁶Cd₂Re₂¹⁸O₇, not only confirm the already known structural phase transitions but also allow us to identify a new characteristic temperature regime around ≈ 80 K, below which the Raman spectra undergo remarkable changes with the development of several sharp modes and mode splitting. Together with the results of the *ab initio* phonon calculations we take these observations as strong evidence for another phase transition to a novel low-temperature crystal structure of Cd₂Re₂O₇.

Primary author: OLEŚ, Andrzej M. (Marian Smoluchowski Institute of Physics, Jagiellonian University, Cracow, Poland)

Co-authors: KAPCIA, Konrad J. (Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland); REEDYK, Maureen (Department of Physics, Brock University, St. Catharines, Canada); HAJIALAMDARI, Mojtaba (Department of Physics, Brock University, St. Catharines, Canada); PTOK, Andrzej (Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland); PIEKARZ, Przemysław (Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland); RAZAVI, Fereidoon S. (Department of Physics, Brock University, St. Catharines, Canada); KREMER, Reinhard K. (Max Planck Institute for Solid State Research, Stuttgart, Germany)

Presenter: OLEŚ, Andrzej M. (Marian Smoluchowski Institute of Physics, Jagiellonian University, Cracow, Poland)