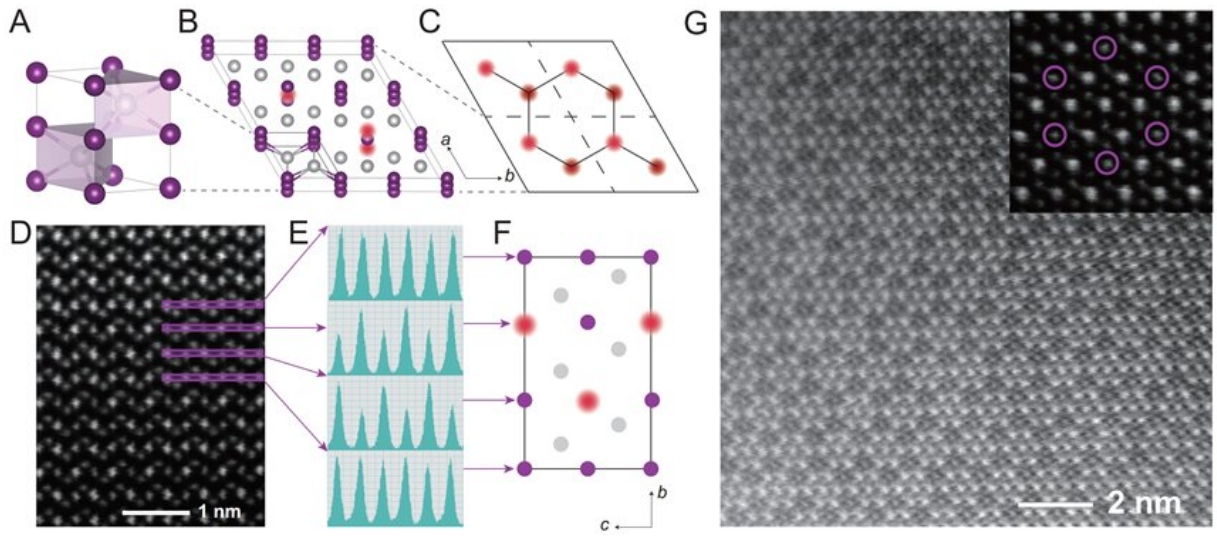
Superconductivity from buckled-honeycomb-vacancy ordering

March 22 2021



Superstructure with BHV ordering. A. NiAs-type primary cell (space group P63/mmc). The point groups at the Ir (purple circles) and Sb (grey circles) sites are D3d and D3h, respectively. B. Crystal structure of Ir16Sb18. Ir vacancies are indicated by red shadowed circles. C. Illustration of BHV ordering seen from the c-axis. Note the Ir and Sb atoms were omitted for clarity. D. High-angle annular dark-field (HAADF) micrograph along the a-axis. E. Intensity line profile of the region marked by the arrows. F. Projection of the BHV superstructure along the a-axis. G. HAADF micrograph of the Ir16Sb18 along the c-axis. The dark sites are the iridium vacancies. The inset shows one honeycomb hexagon at a higher magnification. Credit: ©Science China Press

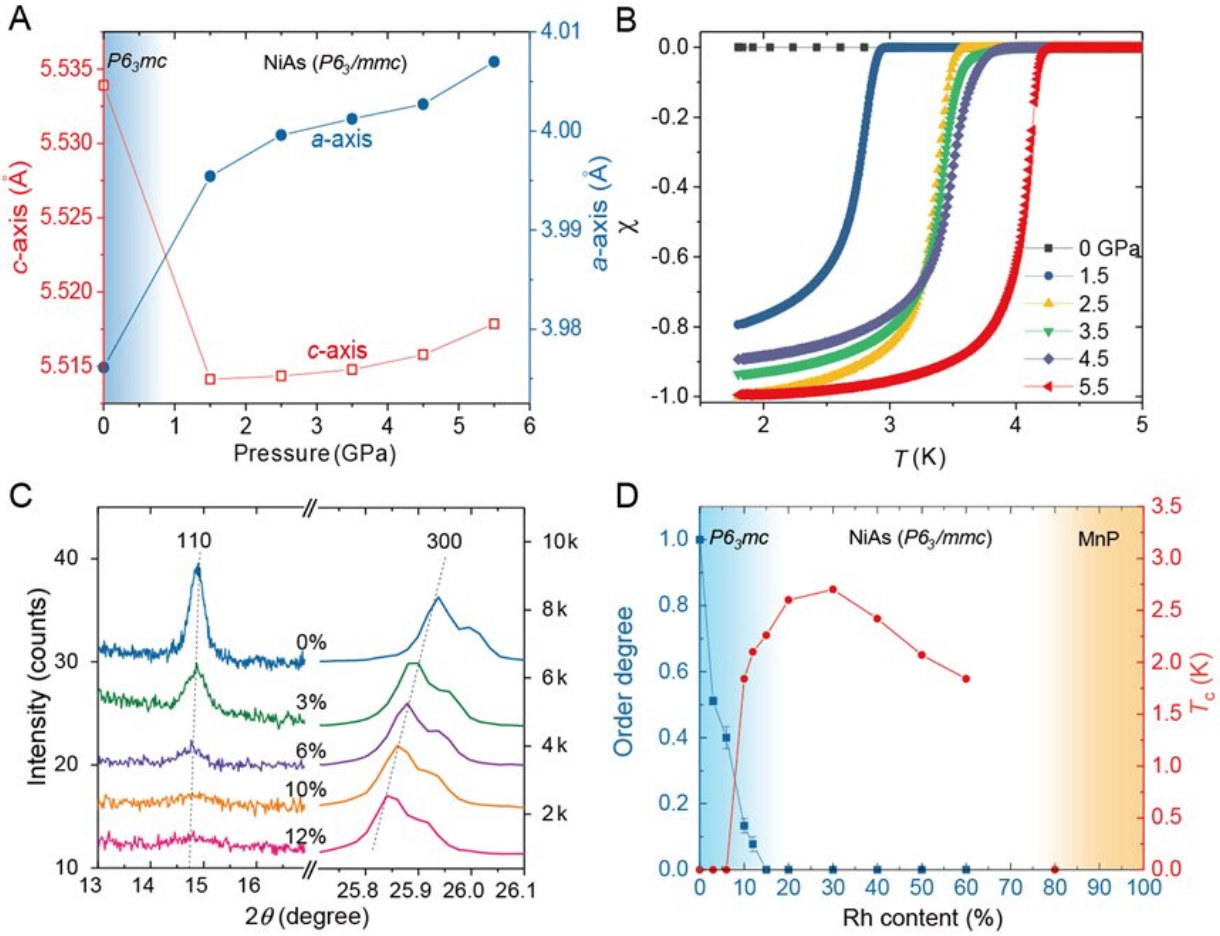
Crystals inherently possess imperfections. Vacancies, as the simplest

form of point defects, significantly alter the optical, thermal, and electrical properties of materials. Well-known examples include color centers in many gemstones, the nitrogen-vacancy center in diamond, vacancy migration in solid-state batteries, and the metal-insulator transition in phase-change materials. The vacancies in these cases are in frame-works with no or weak interactions. However, the role of vacancies in strongly correlated materials is thus far unclear due to the lack of an ideal prototype.

Strongly correlated vacancy ordering has long been anticipated to harbor exotic physics, such as superconductivity. The K-Fe-Se superconductor has been a hot research subject in recent studies for an important reason, viz., the existence of an insulating iron-vacancy-ordering phase. However, this vacancy-ordering phase has been proven to coexist with the superconducting phase at the nanoscale, and is not responsible for the superconductivity. Whether correlated vacancies could become a new type of superconducting parent phase is an unanswered question. Iridates, with comparable and competing energy scales of the on-site Coulomb repulsion, crystal field and spin-orbit coupling, are a platform of rich structures and physical properties.

Recently, a joint research team from Yanpeng Qi group from ShaihaiTech University and Hosono group at the Tokyo Institute of Technology, discover an unprecedented vacancy state in $Ir_{16}Sb_{18}$, forming an extended buckled-honeycomb-vacancy (BHV) ordering. Superconductivity emerges by suppressing the BHV ordering through squeezing of extra Ir atoms into the vacancies or isovalent Rh substitution. The phase diagram reveals that the superconductivity competes with the BHV ordering, which ranks it as the first superconducting parent phase with correlated vacancies. Further theoretical calculations suggest that this ordering originates from a synergistic effect of the vacancy-formation energy and Fermi surface nesting with a wave vector of (1/3, 1/3, 0). The buckled structure breaks

the crystal inversion symmetry and can mostly suppress the density of states near the Fermi level. This study suggests that the ordered vacancy can be a new degree of freedom for the manipulation and study of quantum materials. Further investigation of how the vacancy intertwines with other conventional degrees of freedom like lattice, spin and orbital, and their influence towards the properties of the materials will be fascinating and hold promise for novel discoveries in physics.



Competition between BHV ordering and superconductivity. A. Lattice parameters along the a- and c-axes of Ir1-δSb as the synthesis pressure increased. B. Diamagnetization (calibrated by using Pb as a standard sample) of Ir1-δSb samples synthesized under various pressures. C. The intensity of the Laue reflections 110 (superstructure) and 300 (main structure) at various iso-valent Rh

content. D. Phase diagram of Ir1-xRhxSb. Credit: ©Science China Press

More information: Yanpeng Qi et al, Superconductivity from buckled-honeycomb-vacancy ordering, *Science Bulletin* (2020). DOI: 10.1016/j.scib.2020.12.007

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