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FIRST-PRINCIPLES MATERIALS BY DESIGN FOR THERMODYNAMICALLY STABLE LOW-DIMENSIONAL ELECTRIDES

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Two-dimensional (2D) electrides, emerging as a new type of layered material whose electrons are confined in interlayer spaces instead of at atomic proximities, are receiving interest for their high performance in various (opto) electronics and catalytic applications. A realization of electrides containing anionic electrons has been a great challenge because of their thermodynamic stability. For example, experimentally, only a couple of layered nitrides and carbides have been identified as 2D electrides. We developed a material by design scheme and applied it to the computational exploration of new low-dimensional electrides. Our approach here offers an important alternative that overcomes the current limitation on discovery of new 2D inorganic electrides. By combining the global structure optimization method and first-principles calculations, we identified new thermodynamically stable electrides that are experimentally accessible. Most remarkably, we, for the first time, reveal an effective design rule for 2D electrides. We then discover another new class of electrides, the first electride with nontrivial band topology, based on 1D building block by coupling materials database searches and first-principles-calculations-based analysis. This new class of electrides, composed of 1D nanorod building blocks, has crystal structures that mimic β-$TiCl_3$ with the position of anions and cations exchanged. Unlike the weakly coupled nanorods of β-$TiCl_3$, Cs_3O and Ba_3N retain 1D anionic electron along the hollow inter-rod sites; additionally, strong inter-rod interaction in C_3O and Ba_3N induces band inversion in a 2D superatomic triangular lattice, resulting in Dirac nodal lines. Our work represents an important scientific advancement over previous knowledge of realizing electrides in terms of both materials and design principles, and should interest the communities of catalytic chemistry, surface physics, and structural chemistry, as well as the related engineering disciplines.

Biography

Mina Yoon has received her PhD degree in Theoretical Condensed Matter Physics from Michigan State University. She is a Research Scientist at ORNL and a joint Professor of Physics at UTK. She is a recipient of a Max Planck Fellowship and the Lee Hsun Young Scientist Award from the Institute of Metal Research, Chinese Academy of Science. She has published more than 75 journal papers and has been serving as an Editorial Board Members of international journals and organizer of various international conferences/workshops.

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