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Materials by design for thermodynamically stable 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 atomic proximities, are receiving interest for their high performance in various optoelectronics 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. Here, we report new thermodynamically stable low-dimensional (1D and 2D) electrides by using first-principle global structure optimization method, phonon spectrum analysis, and molecular dynamics simulation. The method was applied to binary compounds consisting of alkaline-earth elements as cations and group VA, VIA, or VIIA nonmetal elements as anions, and further extended to less than ~100 K materials in databases. We demonstrated a new avenue to discover new electrides and provide new design principles, which will significantly boost the discovery of this new class of material with great technical application.

Biography

Mina Yoon received her PhD degree in Theoretical Condensed Matter Physics in 2004, from Michigan State University. She is a Research Scientist at ORNL and a Joint Professor of Physics at University of Tennessee, Knoxville.

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