Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**First-principles Prediction of Thermodynamically Stable Two-Dimensional Electrides**[1] MINA YOON, WENMEI MING, MAO-HUA DU, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States, KI-MOON LEE, Kunsan National University, 558 Daehak-ro, Gunsan, Jeonbuk 573-701, South Korea, SUNG WNG KIM, Sungkyunkwan University, 300 Cheoncheon-dong, Jangan-gu, Suwon, Gyeonggi-do 440-746, South Korea — 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. Experimentally, however, 2D electrides have been only found in a couple of layered nitrides and carbides. Here, we report new thermodynamically stable alkaline-earth based 2D electrides by using a first-principles 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. We revealed that the stability of layered 2D electride structure is closely related to the cation/anion size ratio; stable 2D electrides possess a sufficiently large cation/anion size ratio to minimize electrostatic energy among cations, anions, and anionic electrons. Our work demonstrates a new avenue to the discovery of thermodynamically stable 2D electrides beyond experimental material databases and provides new insight into the principles of electride design.

[1]Research performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility, and supported by the National Research Foundation of Korea funded by the Ministry of Science, ICT and Future Planning.

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Date submitted: 28 Nov 2016 Electronic form version 1.4