

Abstract Submitted
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Design of Inorganic Electrides YUNWEI ZHANG, HUI WANG, YAN-CHAO WANG, YANMING MA, State Key Lab of Superhard Materials, Jilin University — Electrides, in which all of or part of the valence electrons occupy interstitial regions in the crystal and behave as anions, have been synthesized at ambient or high-pressure conditions [1]. Their loosely bound anionic electrons make electrides good candidates for electro-active materials. Here, we report a developed methodology to systematically design electrides for given chemical systems. The new approach is based on the swarm-intelligence CALYPSO algorithm on structure prediction [2] and requires only the chemical compositions to predict the electride phases. In contrast to the traditional ground state structure prediction method where the total energy was solely used as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of given chemical systems. The experimentally known electrides have been successfully reproduced. The results suggested that our approach is reliable and can be widely applied into design of new electrides.

[1] Ma, Y. et al. Transparent dense sodium. *Nature* 485, 182-185 (2009).

[2] Wang, Y., Lv, J., Zhu, L. & Ma, Y. Crystal structure prediction via particle-swarm optimization. *Phys. Rev. B* 82, 094116 (2010).

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