Dsign of Inorganic Electrides ZHANG YUNWEI, PENG FENG, MA
YANMING, Stake Key Laboratory 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 [2-3]
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 result 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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