EVOLUTIONALLY SEARCH WITH DENSITY FUNCTIONAL CALCULATIONS FOR A NEW CLASS OF ONE-DIMENSIONAL *ELECTRIDE*

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An *electride*, a unique material in which electrons serve as anions, has begun to attract attention for its high performances in electronic and catalytic applications. However, the chemically active property of electrides make the synthesis very difficult, and thus finding stable electrides is a big challenge. Based on a dimensional analysis on the stability of electrides [1], we focused on phosphide-based compounds, and we adopted a state-of-the-art theoretical evolutionally search combined with density functional calculations for a new class of electrides; Strontium phosphide in which anionic electrons are ordered in a one-dimensional network (Fig.1) was found [2]. The presence of the one-dimensional electride was proved by the successful synthesis and X-ray diffraction pattern of the compound. However, an interesting discrepancy appears in its electronic property: metal from density functional theory, but insulator from experiment [2]. We analyzed the discrepancy in terms of the inherent instability of one-dimensional metal especially in half-filled systems, and found a gap-opening by introducing electron correlations, which implies the possibility of the one-dimensional electride as a Mott-insulator. Recently, ytterbium antimonide which takes the same crystal structure of the strontium phosphide is found as a Mott-insulating electride [3]. Although a standard density functional calculation is not preferred for correlated systems, the “structure prediction” by evolutionally search combined with density functional probably work well also for such a system because of the energy scale differences between structural changes and electron correlations.

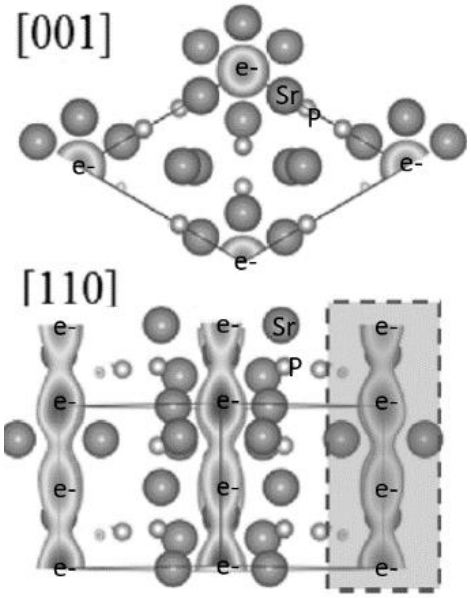

Figure 1 Crystal structure of Sr5P3.

References

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