Supplementary Information (SI) for RSC Advances.
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The respectable reviewer # 2 has suggested to send a supporting document containing the details of the tests for parameter selection, such as cutoff radius and k-point mesh etc for the present calculation. The WIEN2k software is employed in the present work, it is used for performing electronic structure calculations of solids using density functional theory, the tests for parameter selection, such as cutoff radius and k-point mesh, etc in these theoretical calculations are vital for producing accurate and dependable results. Following are the main parameters and their basis:

1) RK_{max} (RMT × K_{max}): It is a product of the smallest muffin-tin radii "RMT" and the maximum reciprocal lattice vector "K_{max}" which is used in the plane wave expansion. The $R \times K_{max}$ affects the precision of plane wave expansion. Its values typically range from 6 to 9 but may vary depending on the desired accuracy and the elements comprised. A greater $R \times K_{max}$ raises the computational cost while generally increasing the accuracy. In the interstitial area, we used plane wells with a cutoff of $RMT \times K_{max} = 8$. The $L_{max} = 8$ and $G_{max} = 14$ were selected as the additional input for the Wien2k package. The Fourier-expanded charge density is shown by G_{max}, and l_{max} was the highest value of the angular momentum vector.

2) Muffin-tin radii (RMT) refers to the spherical regions of an atom when the potential and wavefunctions are thought to be symmetric. RMT must be selected so that the spheres are not overlapping and remain as large as possible to reduce the interstitial region. Yet they must be less for densely packed structures or elements with short atom radii. The values of the muffin radii are 2.01 for K, 2.51 for Th, 2.31 for Sm, 2.0 for Cu, and 1.7 Bohr for S, are selected.

3) K-points: K-points are Brillouin zone points used for reciprocal space integration. The number of k-points must be adequate to accurately sample the Brillouin zone; we used a dense (10 × 10 × 10) k-point grid in the first BZ reciprocal space. The Monkhorst-Pack system is often used to generate k-point grids.

4) The Energy Cut_{off} (E_{max}) relates to the maximum energy limit for plane waves in the basis set. E_{max} must be set high enough to guarantee convergence of total energy along with other properties. Usually, it is linked to the RK_{max} parameter. Convergence criteria apply to self-consistent field (SCF) computations, including total energy, charge density, and forces. These criteria must be strict enough to produce accurate findings. Energy convergence criteria typically range from 10^{-4} to 10^{-6} R_y, while charge density convergence criteria are around 10^{-4} e/a.u. It is decided that -6.0 R_y will serve as the cut-off energy for defining the separation of core-valence states. To ensure proper optimization, force, and stress tensor component criteria must be established. Common force convergence criteria are in the range of 1 mR_y/a.u. When the force convergence threshold reaches roughly 10^{-4} eV/Å the iterations are stopped, and the self-consistent criterion is chosen to have an accuracy of 10^{-6} R_y.

The Exchange-Correlation function describes the energy exchanged inside DFT. The choice is determined by the system being researched. The Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), and hybrid functionals are typically all widely employed. We carefully adjusted these parameters based on the physical and chemical features of the systems being studied using WIEN2k which can provide precise and reliable theoretical modeling.