First Principles Studies of the Dielectric Properties of Cesium Hafnium Chloride (Cs_2HfCl_6) as a Scintillating Material

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Introduction

Cesium Hafnium Chloride or CHC is a material of interest because its inherent scintillating properties, without the need of additional doping. First principles calculations are done using the Vienna Ab Initio Simulation Package (VASP). The dielectric spectrum is rendered in VASP; this makes it possible to perform optical calculations.

Requirements

VASP is a program for modelling atomic scale materials from first principles. In depth calculations require heavy computational resources. Access to a High-Performance Computing (HPC) cluster is suggested to facilitate the additional processing power.

Recommended specifications for intense calculations are as follows: minimum 64 GB of memory per node, minimum 24 core processor per node with faster interconnects (greater than 10 Gbits/s) and minimum 32 to 48 cores with slower interconnects (less than 10 Gbits/s), as well as at least 5 TB of storage space for multiple users to store output.

Results

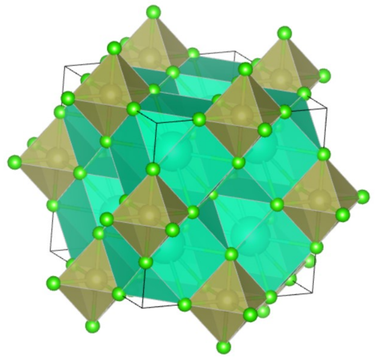

Figure 1 Polyhedral structure of CHC.

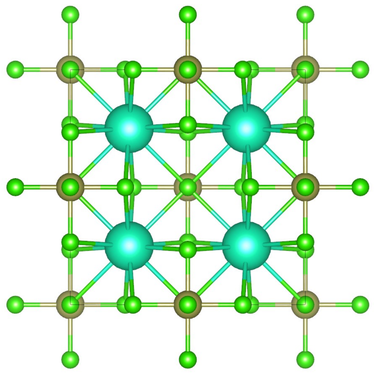

Figure 2 Octahedral tilting of Cs-Cl bond.

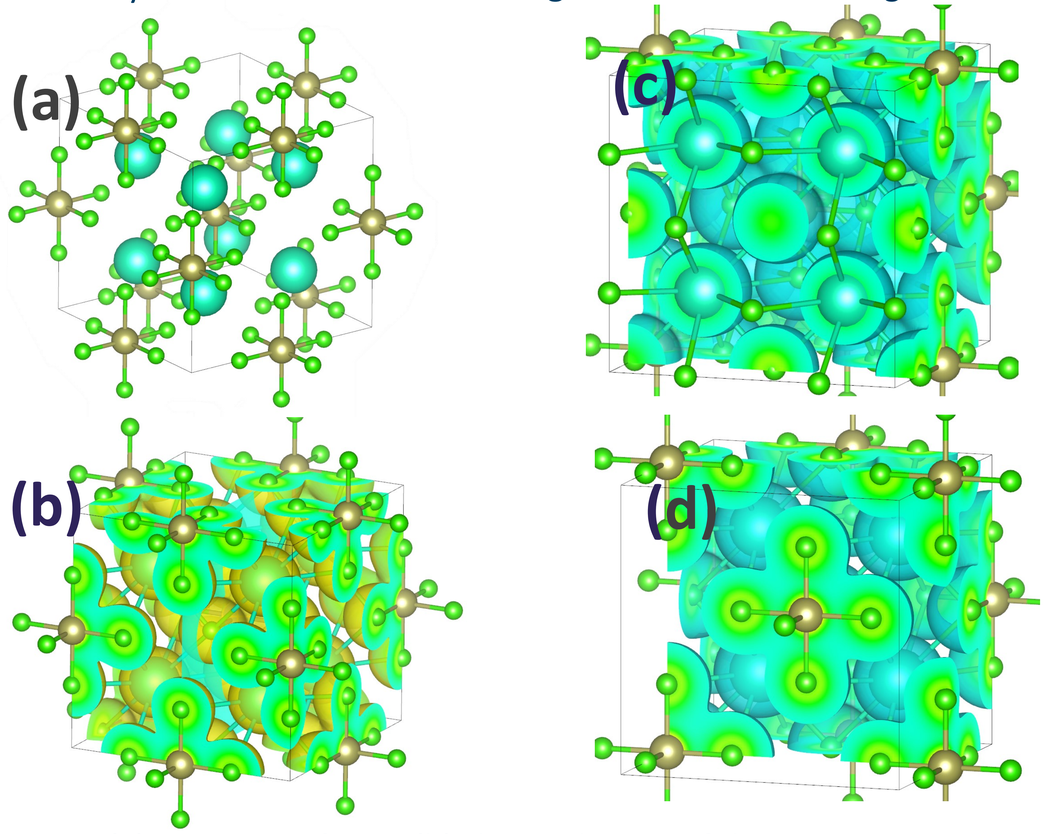

Figure 3 (a) Structure of CHC, (b) charge density of the atoms, (c), and (d) cut isosurface view of charge density.

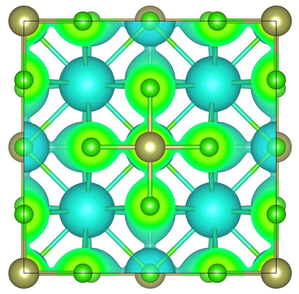

Figure 4 Head on view of charge density without outer bonds.

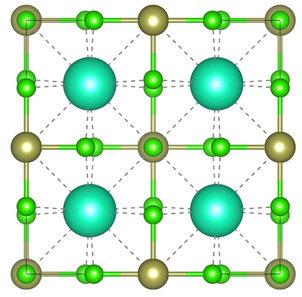

Figure 5 Octahedral tilting of Cs-Cl bond without outer bonds.

Methods

Density Functional Theory (DFT) simulations were performed with VASP 6, using the HSE06-D3 screened hybrid-exchange correlation functional and the PBE generalized gradient approximation functional.

Conclusions

This research is currently ongoing; however, advancements have been made, such as determining the effect of dispersion forces on the material bonds. Optical and electronic effects will be simulated next.

References

Kang, & Biswas, K. (2016). Carrier Self-trapping and Luminescence in Intrinsically Activated Scintillator: Cesium Hafnium Chloride (Cs2HfCl6). *The Journal of Physical Chemistry*, 12187–12195. https://doi.org/10.1021/acs.jpcc.6b02496

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