|  |  |  |  |
| --- | --- | --- | --- |
| Title | Thermodynamic and dynamic stability in a new potential Cs2AgAsCl6 perovskite: insight from DFT study | | |
| Author(s) Name | Tusar Saha, Md. Majibul Haque Babu, Md. Arifuzzaman, Jiban Podder | | |
| Contact Email(s) | [tusar.justphy@gmail.com](mailto:tusar.justphy@gmail.com), [jpodder@phy.buet.ac.bd](mailto:jpodder@phy.buet.ac.bd) | | |
| Published Journal Name | Physical Chemistry Chemical Physics | | |
| Type of Publication | Article | | |
| Volume | 24 | Issue | 43 |
| Publisher | Elsevier | | |
| Publication Date | 11 October 2022 | | |
| ISSN | 1463-9076 | | |
| DOI | <https://doi.org/10.1039/D2CP03152C> | | |
| URL |  | | |
| Other Related Info. |  | | |
|  | | | |

|  |  |
| --- | --- |
| Abstract |  |
| In the present study, we propose a novel type of lead-free double halide perovskite Cs2AgAsCl6 material exhibiting exceptional photovoltaic and photocatalytic properties. Density functional theory (DFT) is employed to investigate the photovoltaic and photocatalytic properties based on several significant properties of the Cs2AgAsCl6 material. The thermodynamic stability of Cs2AgAsCl6 has been confirmed by the enthalpy formation, which is −32.36 eV f.u.−1 Dispersion of phonons near the gamma point confirmed the existence of dynamical stability. The constant value of the heat capacity is 59.45 cal per cell K, which is calculated by the Dulong–Petit limit. The GGA-PBE and HSE-06 functional approaches determined indirect bandgaps of 1.31 and 2.49 eV, respectively, for a semiconductor whose electronic properties revealed photocatalytic efficiency. The effective masses of an electron and a hole are 0.46 *m*e and 0.61 *m*e, respectively, which may enhance the photocatalytic dye degradation owing to their low carrier effective mass. Notably, better photocatalytic properties, *i.e.*, dye degradation, are confirmed by the redox potential. The estimated edge potentials of the conduction band (CB) and valence band (VB) are −0.048 and 2.448 eV, respectively, which are greater than the H+/H2 and O2/H2O potentials. The Cs2AgAsCl6 material reveals an outstanding optical property that is suitable for photovoltaic applications. Therefore, Cs2AgAsCl6 can act as a potential candidate in the field of photovoltaic and photocatalytic applications. | |