

Structural and Optical Properties of Aziridinium Germanium Hybrid Perovskites

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Hybrid halide perovskites containing small organic cations continue to attract attention as semiconducting materials for optoelectronic applications, which make them promising candidates for next-generation photovoltaic and optoelectronic devices. Among them, aziridinium-based perovskites represent an emerging class of compounds with distinctive structural and optoelectronic properties, enabling the formation of stable three-dimensional perovskite frameworks.[1, 2] In the present work, a series of germanium-based hybrid perovskites with the general formula (AzrH)GeX₃ (X = Cl, Br) were synthesized and comprehensively studied. Single-crystal X-ray diffraction analysis revealed that (AzrH)GeCl₃ crystallizes in the *Pnma* space group and (AzrH)GeBr₃ crystallizes in *R3m* space group at room temperature and are characterized by a non-centrosymmetric crystal structure – a distinctive feature that may open opportunities for nonlinear optical applications. Differential scanning calorimetry (DSC) and variable-temperature X-ray diffraction measurements indicate the presence of temperature-induced phase transitions. Optical diffuse reflectance spectroscopy was used to determine the band gap values by the Kubel'ka-Munk method, which were found to be 3.18 eV for (AzrH)GeBr₃ and 3.87 eV for (AzrH)GeCl₃. These results allow us to classify the materials as wide-band-gap semiconductors. The obtained data extend the family of aziridinium-based perovskites and demonstrate that germanium substitution leads to significant changes in the structure and electronic characteristics compared to their lead and tin analogues.

1. Petrosova, H. R. et al. Chem. Commun. 2022, 58, 5745–5748.
2. Kucheriv, O. I. et al. Inorg. Chem. Front. 2023, 10, 6953–6963.

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