Accurate band-gap database for semiconducting inorganic materials: beyond the level of PBE

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Semiconducting inorganic materials with band gaps ranging between 0 and 5 eV constitute major components in electronic, optoelectronic and photovoltaic devices. In particular, semiconductors are used in various fields because of the unique characteristics of materials. For instance, in photovoltaic devices, materials with a direct E_g of ~1.3 eV, corresponding to the Shockley-Queisser limit, are favored as photo-absorbers that maximize the solar-cell efficiency. In power electronics, semiconductors with $E_g \geq 3$ eV are employed to sustain high electric fields. Currently, there are several inorganic material databases providing band gaps based on the Generalized Gradient Approximation (GGA) functional, including Materials Project [1], the Automatic Flow of Materials Discovery Library (AFLOWLIB) [2], the Open Quantum Materials Database (OQMD) [3], and the Joint Automated Repository for Various Integrated Simulations (JARVIS) (the JARVIS provides E_g based on meta-GGA, which significantly improves the accuracy) [4]. However, they suffer from computational limitations such as band-gap underestimation and metastable magnetism. In this study, we present a computational database of band gaps for 10,481 materials compiled by applying a hybrid functional and considering the stable magnetic ordering [5]. For benchmark materials, the root-mean-square error in reference to experimental data is 0.36 eV, significantly smaller than 0.75-1.05 eV in the existing databases. . Furthermore, we classify many small-gap materials that are misclassified as metals in other databases. By providing accurate band gaps, the present database will be useful in screening materials in diverse applications.

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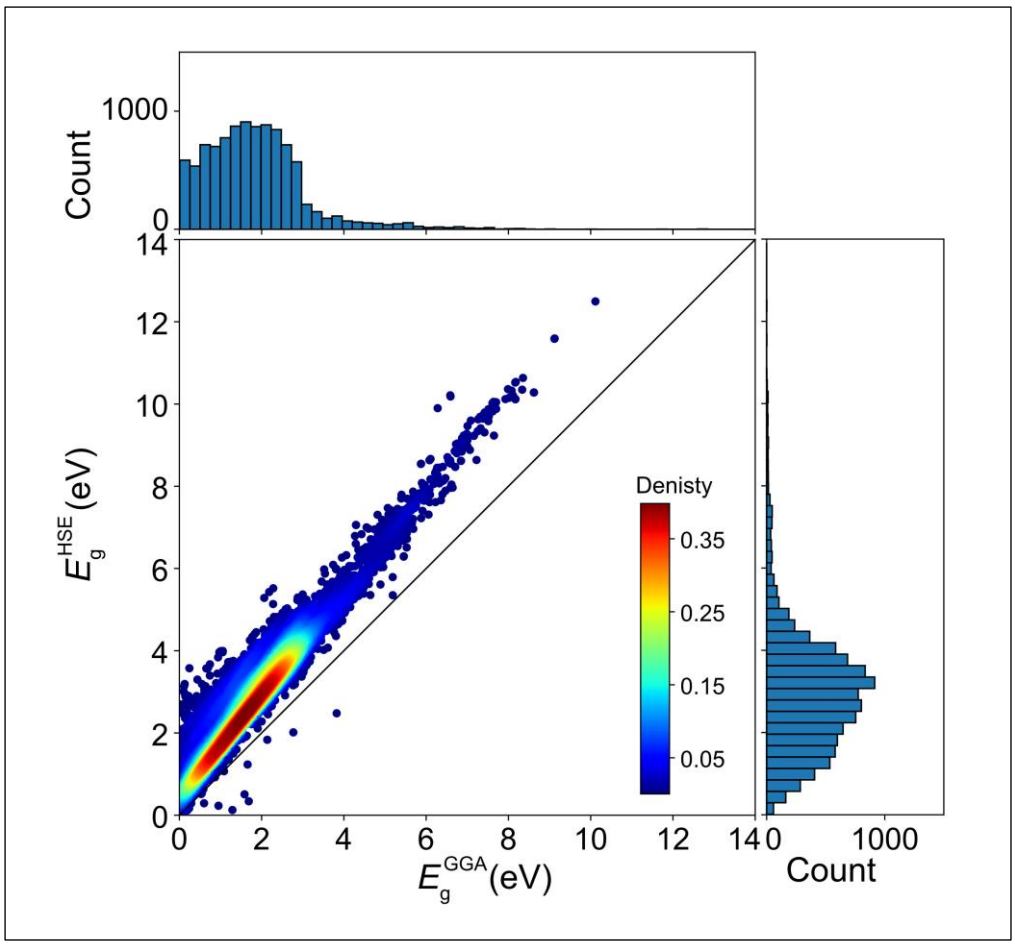

Fig.1: Distribution of $E_g{}^{GGA}$ and $E_g{}^{HSE}$. Top and right are occurrence histograms of $E_g{}^{GGA}$ and $E_g{}^{HSE}$, respectively