

Energy band gap modeling of doped bismuth ferrite multifunctional material using gravitational search algorithm optimized support vector regression

ABSTRACT

Bismuth ferrite (BiFeO_3) is a promising multiferroic and multifunctional inorganic chemical compound with many fascinating application potentials in sensors, photo-catalysis, optical devices, spintronics, and information storage, among others. This class of material has special advantages in the photocatalytic field due to its narrow energy band gap as well as the possibility of the internal polarization suppression of the electron-hole recombination rate. However, the narrow light absorption range, which results in a low degradation efficiency, limits the practical application of the compound. Experimental chemical doping through which the energy band gap of bismuth ferrite compound is tailored to the desired value suitable for a particular application is frequently accompanied by the lattice distortion of the rhombohedral crystal structure. The energy band gap of doped bismuth ferrite is modeled in this contribution through the fusion of a support vector regression (SVR) algorithm with a gravitational search algorithm (GSA) using crystal lattice distortion as a predictor. The proposed hybrid gravitational search based support vector regression HGS-SVR model was evaluated by its mean squared error (MSE), correlation coefficient (CC), and root mean square error (RMSE). The proposed HGS-SVR has an estimation capacity with an up to 98.06% accuracy, as obtained from the correlation coefficient on the testing dataset. The proposed hybrid model has a low MSE and RMSE of 0.0092 eV and 0.0958 eV, respectively. The hybridized algorithm further models the impact of several doping materials on the energy band gap of bismuth ferrite, and the predicted energy gaps are in excellent agreement with the measured values. The precision and robustness exhibited by the developed model substantiate its significance in predicting the energy band gap of doped bismuth ferrite at a relatively low cost while the experimental stress is circumvented.

Keyword: Bismuth ferrite; Support vector regression; Energy band gap; Gravitational search algorithm; Hybridization