First-Principles calculations on donor doping on multiferroic properties of $BiFeO_3$

Tokyo Institute of Technology, Innovator and Inventor Development Platform
Dan Ricinschi

Purpose Clarify the impact of donor doping on local and global magnetic moment of $BiFeO_3$ supercells as well as on its electronic and ferroelectric properties.

Result It appears possible to enhance the magnetization of BiFeO3 without significantly affecting its ferroelectricity, with an added bonus of tuning its band gap so that it becomes suitable for photovoltaic applications.

Computing system: VCC (+HCC)

node-hour	about 600 node-hour of VCC
memory used	up to 50 GB
parallelize	up to 4 nodes of VCC