

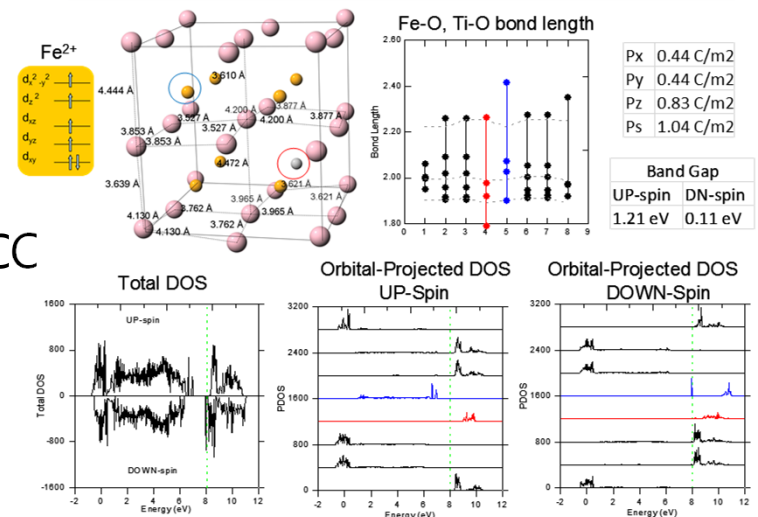
# First-Principles calculations on donor doping on multiferroic properties of $\text{BiFeO}_3$

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**Purpose** Clarify the impact of donor doping on local and global magnetic moment of  $\text{BiFeO}_3$  supercells as well as on its electronic and ferroelectric properties.

**Result** It appears possible to enhance the magnetization of  $\text{BiFeO}_3$  without significantly affecting its ferroelectricity, with an added bonus of tuning its band gap so that it becomes suitable for photovoltaic applications.

**Ti-doped BFO with space-modulated bond lengths**



**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