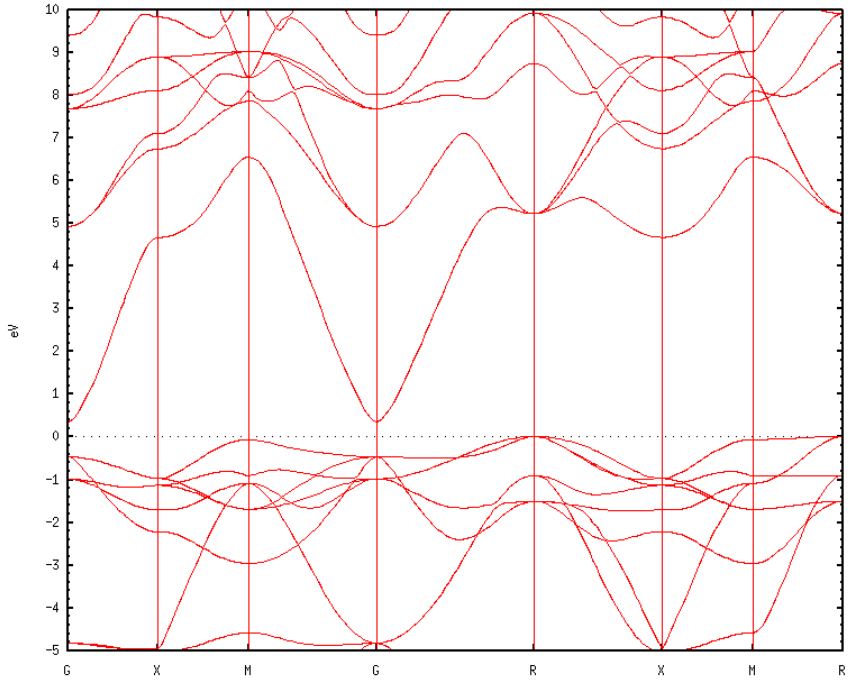
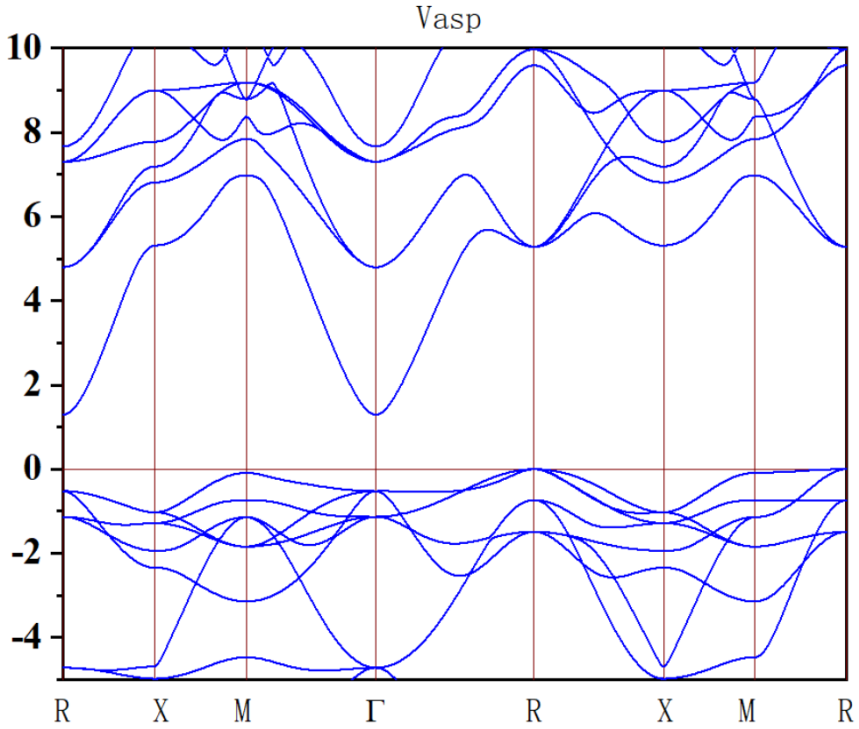
OpenMX: LDA

Ba	Ba10.0-s3p2d1	Ba_CA19
Sn	Sn7.0-s2p2d1	Sn_CA19
O	O5.0-s2p2d1	O_CA19

The result shown by Dr. Zuzhang Lin





The overall feature of the band structure of BaSnO3 calculated by both the codes looks similar. The band gap by OpenMX is ~ 0.4 eV, which seems to be smaller than that by VASP. However, the band structure by calculated by VASP, shown at https://materialsproject.org/materials/mp-3163/ also exhibits the band gap of 0.395 eV.