Phase transitions in perovskite oxides from first-principles

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Introduction:

Perovskite oxides ABO_3 are interesting, both from theoretical and application point of view. Perovskites are used as ferroelectrics ($BaTiO_3$, $PbTiO_3$) and dielectrics ($CaTiO_3$). They can be potentially used as proton conductors ($SrCeO_3$) or multiferroics ($BiFeO_3$). The colossal magnetoresistance ($Pr_{1-x}Ca_xMnO_3$) and superconductivity ($SrTiO_3$) have also been observed in these systems. Important in this group are bismuth-based compounds $BiMO_3$ (M= Al, Ga, In, Fe, Mn, Co, Ni) which have similar ferroelectric properties to those based on $PbTiO_3$, but without harmful effects on enviroment caused by lead. The second important feature of these compounds is coexistance of ferroelectricity and magnetism (multiferroism). Among all multiferroics, $BiFeO_3$ is the only one in which both phenomena appear above room-temparature. The main obstacle in industrial applications are large leakage currents caused by oxygen vacancies. To reduce oxygen vacancies solid solutions are formed e.g. $BiFeO_3$-$LaFeO_3$. However, this leads to phase transition from ferro- to paraelectric phase.

Aim and methods:

The main purpose of research is to investigate phase transitions in $BiMO_3$ (M= Al, Ga, In, Fe, Mn, Co, Ni) and solid solutions $BiFeO_3$-ABO_3 (A=RE, B=TM) based on density-functional theory calculations. The electronic structure, lattice dynamics and ferroelectric and magnetic properties of aforementioned systems will be investigated. The calculations will be performed by using both commercial (VASP) and open-source (Quantum-Espresso, Abinit, OPENMX) codes.