THE MATERIAL PROPHET PROJECT

The central idea of the Material Prophet program project is to make DFT ab-initio calculations as easily accessible to the widest audience possible, including new users who know little about the details of ab-initio computational methods and crystallography but just want to get quick estimates about common material properties as rapidly and as easily as possible (this contrasts with existing softwares such as those by QuantumWise, SCM and Material Design which still require users to be expert in DFT calculations and offer lots of advanced functionalities). The program would be structured in the form of a “Material properties calculator” with graphical user interface such that, starting from the chemical composition of the repeating unit of the crystal structure under investigation (e.g. CaTiO3 for Perovskite), the program is first able to predict automatically the crystal structure information (space group, atom positions, lattice parameters….) of the most stable phase of the material under given external pressure, and to then calculate the desired material properties of this phase such as optical or mechanical properties. The program would make use of the QUANTUM ESPRESSO DFT code for performing such calculations from first-principles, using several pre-defined sets of parameters such as plane-wave cutoff, kgrid size and pseudopotential type depending on the desired accuracy of the calculation, such that the unfamiliar user does not have to worry about the physical meaning of such parameters and can just rely on the pre-defined settings corresponding to each level of accuracy as well as most of the default settings in Quantum Espresso. In fact the whole package could one day in future be framed in the form of a simple mobile app that can be run both on computers as well as phones. I've been trying to do such crystal structure prediction with Quantum Espresso recently, and simply by relaxing the crystal structure starting from a random guess for the atom positions and lattice parameters in a general triclinic setting, it was able to correctly predict all the stable high-pressure phases of silicon using the "vc-relax" command several times to relax both the atom positions, lattice vectors and lattice parameters simultaneously whilst minimising the enthalpy at the same time (the thermodynamic requirement for phase stability under fixed external pressure and at zero temperature). The only problem is that the program has to perform this relaxation for a varying number of atoms in the unit cell and determine which configuration gives the lowest enthalpy/atom since as far as I know there isn't any way to predict the number of atoms in the unit cell a priori. I know of another program which already does crystal structure prediction called USPEX, but as far as I know it doesn't offer an easy and intuitive GUI for non-specialists to use. Finally, once the approximate atom positions and lattice vectors have been obtained at the end of the relaxation run, an external library such as SPGLIB can be used to refine the crystal structure and identify the space group matching the relaxed crystal structure most closely. In this way the Material Prophet program could serve as a great tool for discovering new materials or new high-pressure phases with desired properties (hence the name of the program).

The diagrams in the next page show the appearance of the program which I would envisage. A good summary of common material properties that could be included in the Material

Prophet calculator can be found here:
https://en.wikipedia.org/wiki/List_of_materials_properties

In addition the program could include routines for performing other common calculations that can be implemented with Quantum Espresso and associated packages, such as thermodynamic properties calculations, phonon dispersion curves and band structure calculations.

1) INITIAL WINDOW TO DEFINE CRYSTAL STRUCTURE

Please enter the chemical composition/formula of the repeating unit in your crystal structure (for example CaTiO3 for perovskite or Si for silicon):

SiO2

Please enter external pressure which should be applied to the crystal: (in kbar)

100

Desired accuracy of the calculation:

Fast	Normal	Accurate

(e.g. fast would correspond to ecut=20 Ry and kgrid=4x4x4, while Accurate would correspond to ecut=40 Ry and kgrid=16x16x16)

Install Quantum Espresso automatically

Enter crystal structure information manually

Calculate most stable crystal structure at given pressure

2) WINDOW SHOWING RESULTS OF RELAXATION RUN AND DEFINING MATERIAL PROPERTIES THAT NEED TO BE CALCULATED

Visualisation of caulcated crystal structure (embedding an external crystal visualization program)

Crystallographic properties of calculated crystal structure (e.g. lattice parameters, lattice vectors, atom positions, Bravais lattice, space group etc....)

Calculate the following material properties:

Mechanical properties Tab | Optical properties Tab | Thermodynamic properties tab | Phonons | Bandstructure | etc.....

☐ Check-boxes for each material property that the user wants
☐ to calculate
☐

Desired accuracy of the calculation:

Fast	Normal	Accurate

Calculate properties