RESEARCH FIELD:
Quantum-mechanical modeling of crystalline solids, with reference to minerals

RESEARCH TOPIC:
Structural, vibrational, thermo-elastic and thermodynamical properties of minerals, from *ab initio* quantum-mechanical simulations

PARTICIPANTS AND COLLABORATIONS:
Mauro Prencipe, Marco Bruno, Marco Rubbo, Walter Vanzetti. In recent years the group has enlisted the help of PhD students is the local school, is active in other schools at other universities (Perugia and Genoa).

RESEARCH DESCRIPTION:
Researches in this field concern the *ab initio* quantum-mechanical simulations of the structure and of the vibrational and thermo-elastic properties of crystalline materials, with particular reference to minerals. The computational technique results to be particularly useful, and complementary with respect to the experimental ones, in the estimation of the elastic properties of materials at high temperature and pressure conditions, in view of the difficulties frequently encountered in the accurate experimental measurements of such quantities at extreme thermo-baric conditions. Results from such researches have important implications in (*i*) the geodynamical modeling of processes occurring at the level of Earth's mantle; (*ii*) the estimation of thermodynamical properties of phases and phase equilibria among minerals at variable pressure and temperature, ranging from typical crustal to lower mantle conditions; (*iii*) the interpretation of the experimental results from the IR and Raman vibrational spectroscopies. Moreover, the *ab initio* computational approach allows for the interpretation of the phenomena, and of the observed properties, within a physically and chemically grounded theoretical framework, thus potentially enlarging the basic knowledge in the field of material science. Among the mineral phases under investigation there are diamonds; various silicates like beryl, pyroxenes, sheet silicates, perovskites and post-perovskite; carbonates like calcite, aragonite and dolomite; phosphates like apatite and carbo-apatite, and oxides like periclase and Fe-periclase.

LABORATORIES OF THE DST IN USE:
High performance parallel computing cluster

RESEARCH PRODUCTS:
The recent most significant and representative scientific publications are:
Vibrational spectroscopies:

- Prencipe M, Mantovani L, Tribaudino M, Bersani D & Lottici P (2012). The Raman spectrum of diopside: a comparison between ab initio calculated and experimentally measured frequencies. *European Journal of Mineralogy*, **24**, 457–464.
- Prencipe M (2012). Simulation of vibrational spectra of crystals by ab initio calculations: an invaluable aid in the assignment and interpretation of the Raman signals. The case of jadeite ($NaAlSi_2O_6$). *Journal of Raman Spectroscopy*, **43**, 1567–1569.
- Prencipe M, Noel Y, Bruno M & Dovesi R. (2009). The vibrational spectrum of lizardite-1*T* [$Mg_3Si_2O_5(OH)_4$] at the Γ point: A contribution from an ab initio periodic B3LYP calculation. *American Mineralogist*, **94**, 986–994.

Thermo-elastic properties of minerals:

- Ungureanu CG, Cossio R & Prencipe M (2012). An Ab-initio assessment of thermo-elastic properties of $CaCO_3$ polymorphs: Calcite case. *Calphad*, **37**, 25–33.

- Scanavino I, Belousov R & Prencipe M (2012). Ab initio quantum-mechanical study of the effects of the inclusion of iron on thermoelastic and thermodynamic properties of periclase (MgO). *Physics and Chemistry of Minerals*, **39**, 649–663.
- Prencipe M, Scanavino I, Nestola F, Merlini M, Civalleri B, Bruno M & Dovesi R. (2011). High-pressure thermo-elastic properties of beryl ($Al_4Be_6Si_{12}O_{36}$) from ab initio calculations, and observations about the source of thermal expansion. *Physics and Chemistry of Minerals*, **38**, 223–239.
- Prencipe M & Nestola F (2006). Minerals at high pressure. Mechanics of compression from quantum mechanical calculations in a case study: the beryl ($Al_4Be_6Si_{12}O_{36}$). Physics and Chemistry of Minerals, 34, 37–52.

Solid solutions and order/disorder phenomena in minerals:

- Zucchini A, Prencipe M, Comodi P & Frondini F (2012). Ab initio study of cation disorder in dolomite. Calphad, **38**, 177–184.

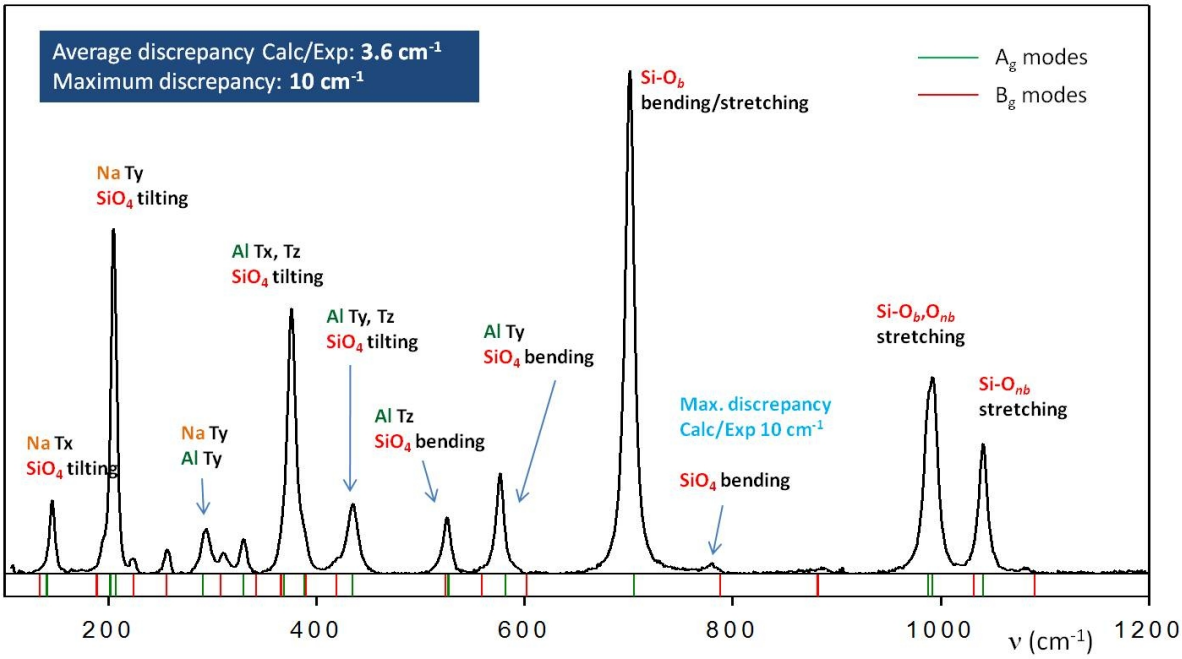

Figure 1: Experimental Raman spectrum of jadeite; correspondence with the calculated frequencies, and attributions of the Raman signals to specific vibrational modes.

GROUP CONTACT: Prencipe Mauro