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Crystal17: A Modern Tool for Ab Initio Solid State Chemistry & Physics

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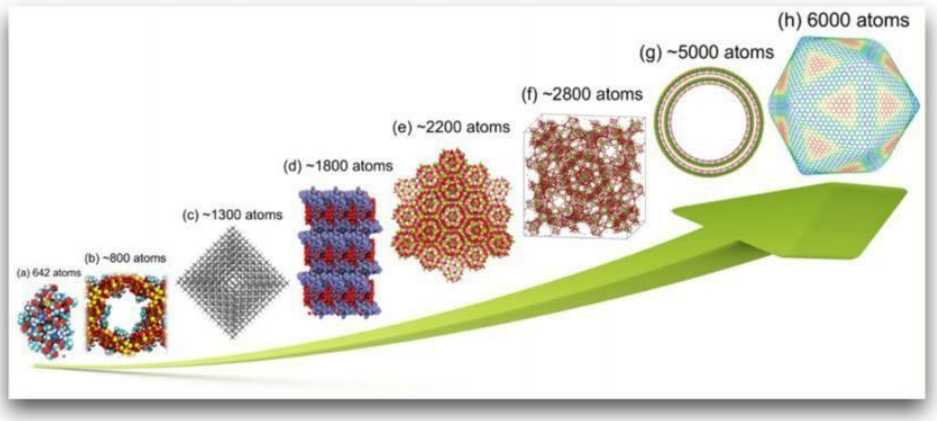
ABSTRACT

The CRYSTAL *ab initio* package for solid state chemistry and physics is presented. First, the theoretical background is shortly recovered to allow for a better understanding of the limitations and peculiarity of the code. Then, some features are discussed with reference to some applications of both fundamental and technological interest. In particular:

- the massive parallel implementation of the code that allows for the modeling of realistic systems;
- the frequencies calculation complemented by the IR and Raman spectra reconstruction;
- the recent transport properties algorithm as applied to derive the thermoelectric performance of several materials (InGaN and Half-Heusler alloys, nanotubes, etc.)
- the new extension of the topological analysis of the charge density to ƒ– and *g*– type basis functions which opens the way to the study of lanthanide and actinide compounds.



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