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Phase-transition studies at the Bilbao Crystallographic Server

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The Bilbao Crystallographic Server (www.cryst.ehu.es) is a free web site with crystallographic databases and programs. The server is built on a core of databases that contain crystallographic data of space groups, magnetic space groups, subperiodic groups and their symmetry relations. Parallel to the crystallographic software we have developed specialized tools for the analysis of complex solid-state physics and structural chemistry problems. The aim of this contribution is to report on databases and computer programs of the server that facilitate complete and thorough phase-transition studies. Starting from the experimental structures of the high- and low-symmetry phases the program STRUCTURE RELATIONS studies the crystal-structure relationship between two phases. It is characterized by a global distortion that, in general, can be decomposed into homogeneous strain and atomic displacement field. The program AMPLIMODES [2] performs the decomposition of the global distortion into symmetry-mode contributions, and the determination of the corresponding polarization vectors. This type of analysis separates the correlated atomic displacements that are fundamental for the phase stability, the so-called primary modes, from the weaker distortions of limited relevance for the transition mechanism. The server also offers online tools for the evaluation of the pseudosymmetry of a given structure with respect to a supergroup of its space group [3]. The detection of structural pseudosymmetry as the consequence of a small distortion of a higher symmetry is a powerful method for the prediction of new ferroic materials. Recently, computer databases and tools for the analysis of magnetic phase transitions have been implemented. Case studies will accompany the presentation of the programs offered by the Bilbao Crystallographic Server and will illustrate their capacities and efficiency in phase-transition studies.

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