World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

# Describing the Fine Electronic Structure and Predicting Properties of Materials with ATOMIC MATTERS Computation System

**Authors :** Rafal Michalski, Jakub Zygadlo

**Abstract :** We present the concept and scientific methods and algorithms of our computation system called ATOMIC MATTERS. This is the first presentation of the new computer package, that allows its user to describe physical properties of atomic localized electron systems subject to electromagnetic interactions. Our solution applies to situations where an unclosed electron 2p/3p/3d/4d/5d/4f/5f subshell interacts with an electrostatic potential of definable symmetry and external magnetic field. Our methods are based on Crystal Electric Field (CEF) approach, which takes into consideration the electrostatic ligands field as well as the magnetic Zeeman effect. The application allowed us to predict macroscopic properties of materials such as: Magnetic, spectral and calorimetric as a result of physical properties of their fine electronic structure. We emphasize the importance of symmetry of charge surroundings of atom/ion, spin-orbit interactions (spin-orbit coupling) and the use of complex number matrices in the definition of the Hamiltonian. Calculation methods, algorithms and convention recalculation tools collected in ATOMIC MATTERS were chosen to permit the prediction of magnetic and spectral properties of materials in isostructural series.

**Keywords :** atomic matters, crystal electric field (CEF) spin-orbit coupling, localized states, electron subshell, fine electronic structure
**Conference Title :** ICSRD 2020 : International Conference on Scientific Research and Development
**Conference Location :** Chicago, United States
**Conference Dates :** December 12-13, 2020