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DFT techniques for interpretation and solution of significant practical problems

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Significant examples of advances in prediction of properties for practical materials and for understanding of fundamental properties, guided by use of DFT computational techniques, are presented. One example is from the field of battery materials for electric vehicles, where understanding of surface phenomena via a combination of multiple experimental techniques and extensive DFT calculations of electronic band structures, is leading to significantly improved cycle life of battery materials. The other example is from the field of superconductivity. Again, interpretation and analysis of results obtained using advanced experimental techniques, interpreted with the assistance of DFT calculations, reveals that crystal symmetries of superconductors are different from the general types normally attributed to them. The insight gained from precise DFT calculations is unparalleled and accelerates research progression. The importance of calibration for accurate and realistic DFT approaches to modelling, combined with regular experimental validation, cannot be overstated.

Primary author(s) : Prof. ALARCO, Jose (Queensland University of Techology); Prof. MACKINNON, Ian (Queensland University of Technology)

Presenter(s) : Prof. ALARCO, Jose (Queensland University of Techology)

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