MODELLING of POINT DEFECTS in MATERIALS: ACHIEVMENTS, CHALLENGES and PROSPECTS

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We will summarise briefly how the use of modelling techniques can yield unique information on structure, dynamics, and energies of point defects in a wide range of materials, thereby illuminating and assisting experimental studies. Our discussion will concentrate on the following approaches and systems:

(i) The application of the Mott Littleton Method with applications to defects in oxides.
(ii) The application of periodic boundary condition's electronic structure, techniques, illustrated by reference to work on semiconductors including transparent semi-conducting systems.
(iii) The application of Quantum Mechanical/ Molecular Mechanical (QM/MM) techniques, illustrated by modelling of defects in nitrides
(iv) The role of molecular dynamics techniques

We will review the strengths and challenges of the different approaches and will discuss their application to other areas of defect chemistry and physics. We will conclude with a discussion of prospects for the field.