TCM PUBLICATIONS 1997


P.D. HAYNES and M.C. PAYNE “Localised spherical-wave basis set for O(N) total-energy pseudopotential calculations” Computer Physics Communications 102, 17-27 (1997).

V. HEINE “The role of computer experiments in mineralogy: an introduction to the first Kiel workshop on the application of computer simulation to mineralogy” 1st Kiel Workshops: Lecture Notes and Abstracts, B. Winkler ed., Kiel University (1997).


R. SHAH, J.D. GALE and M.C. PAYNE “Comparing the acidities of zeolites and SAPOs from first principles” Chemical Communications 1, 131-132 (1997).


