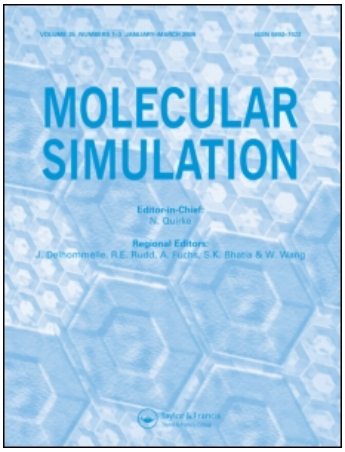

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Calcite and related materials: Growth and dissolution

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CALCITE AND RELATED MATERIALS: GROWTH AND DISSOLUTION

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Calcium carbonate is one of the most widespread sedimentary minerals, commonly found as one of the three phases: calcite, aragonite and vaterite, although several meta-stable anhydrous and hydrous phases are also known. The calcite polymorph is an important rock-forming mineral and is the stable phase in ambient conditions. In addition to the pure calcium form, a host of different cations can be incorporated in the calcite structure and several carbonates are known to crystallise in the rhombohedral calcite form, of which dolomite, an ordered Mg–Ca carbonate, is probably the best known and whose omnipresence in the environment despite little or no formation in present marine environment, is something of an enigma. Carbonate crystal growth and dissolution is a major theme of much recent computational and experimental research.

The formation of calcium carbonate deposits is also a major domestic and industrial problem, from scale formation in kettles and central heating systems to industrial boilers and oil transportation pipes. Hence, a great deal of work has been devoted to finding inhibitors of carbonate growth. In addition, calcite is an important biological material, e.g. as a composite in skeletons and shells. Although much recent work has concentrated on calcite (and to a lesser extent the other phases of calcium carbonate) because of their obvious importance in biology and geology, more and more effort is also being spent on the investigation of other materials containing inorganic molecular ions, such as sulphates, nitrates

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and phosphates. A meeting was held at the University of Reading in January 2001, offering a chance for simulators and experimentalists in different disciplines to present recent work in this area, discuss common problems and encourage more interaction between theory and experiment in this field. We are grateful to CCP5 for sponsorship of this meeting and to Dr R.A. Jackson for his help with the organisation. All participants were invited to contribute to this present issue of Molecular Simulation and we would like to thank Professor C.R.A. Catlow for arranging the opportunity to have these contributions published here.