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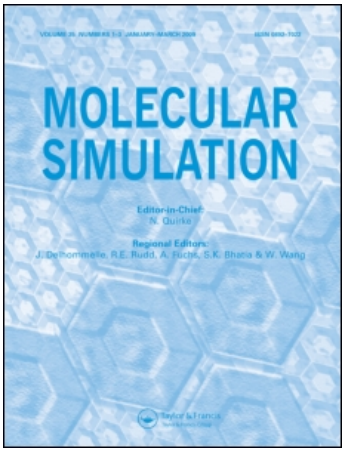

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W. Smith

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Guest Editorial: DL_POLY–applications to molecular simulation II

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This issue of *Molecular Simulation* is a collection of articles derived from the application of the molecular dynamics simulation package known as DL_POLY, which has been a publicly available tool for academic research now for 10 years. It follows on from a previous issue of *Molecular Simulation* in 2002 (*Molecular Simulation* 2002, Vol. 28 (5), pp. 385–471) which provided an overview of the scientific areas DL_POLY was employed in at the time. Now as then, it is clear that the package finds application across a diverse range and has become a valued research tool with a significant number of research groups.

The articles presented here begin with a short description of the structure of the DL_POLY code by the current custodians of the package, W. Smith and I. Todorov, followed by an intriguing article from M. Dove's eMinerals project on how DL_POLY_3 fits into an integrated grid environment, thereby serving a wide ranging project.

Applications of DL_POLY in the biological area are exemplified by the articles from P. Chau and C.W. Yong on protein unbinding and superoxide dismutases respectively.

The structure of crystals is the subject of contributions from P. Bordat *et al.* and S.L. Price *et al.* The former is concerned with solid–solid phase transitions and the latter with issues of polymorphism in molecular crystals. These contributions are complemented by the article from S. Alavi *et al.* on the melting of polyatomic molecular and ionic crystals and nanoparticles and the article on polymer simulations from D. Adolf *et al.*

The properties of liquids and solutions are represented by the article form R.M. Lynden-Bell on the sensitivity of liquid structure to the interaction model, and another from R. Ayala *et al.* on the solvation of the bromide ion in acetonitrile.

DL_POLY has often found application in the study of glasses and two contributions exemplify this. The first is from M. Menziani *et al.* on rationalising the properties of multicomponent glasses and the second on the slow dynamics of glass forming materials is from F. Affouard *et al.*

The large system sizes possible with DL_POLY_3 has made it a useful tool for radiation damage studies. An example of such work is given by R. Devanathan *et al.* in their study of uranium recoil in zircon.

Interfaces and films are represented by three articles. P. Martin has used DL_POLY to look at inorganic interfaces (P. Martin *et al.*), while D. Willock has examined the structure of organosilane film coatings (D. Willock *et al.*). F. Bresme has examined the physics of Newton black films (F. Bresme *et al.*).

The contributions end with an article by J. Elliot *et al.* on the adaptation of DL_POLY for dissipative particle dynamics studies of mesoscopic systems.

The articles gathered here show the versatility of the DL_POLY package and the ingenuity of its users in equal measure. It is extremely gratifying to the authors of the package that it has helped to stimulate so much research, often into areas unimagined by the authors. It is a pleasure to thank the contributors to this special issue for their excellent articles and for promoting the use of DL_POLY so effectively.

W. Smith
Guest Editor

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