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Guest editorial

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Guest editorial

This issue of Molecular Simulation contains contributions from participants at the 2004 Annual Meeting of the American Institute of Chemical Engineers. The Meeting was held in Austin Texas, 7–12 November. The papers represent some of the best work presented at the meeting in the ‘Computational Molecular Science and Engineering Forum’ and the ‘Issue in Carbon Nanotubes sessions’. The papers selected for this issue cover a wide

range of topics including quantum mechanical estimation of rate constants, statistical mechanical molecular dynamics and Monte Carlo, mesoscopic modeling of biomolecules, and experimental synthesis of carbon nanotubes.

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