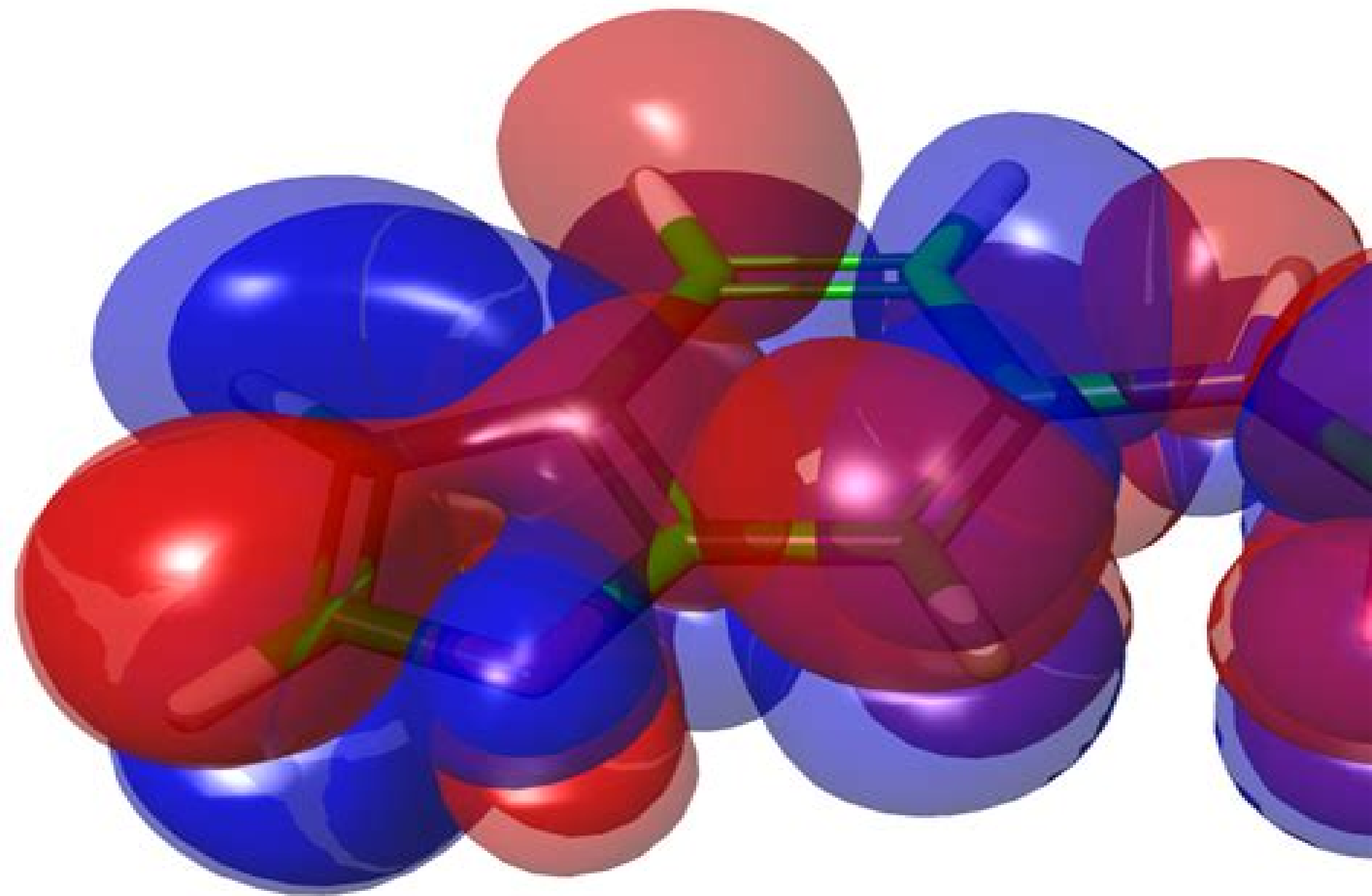




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Materials Informatics I Kunal Roy, Arkaprava Banerjee, 2025-05-10 This contributed volume explores the integration of machine learning and cheminformatics within materials science focusing on predictive modeling techniques It begins with foundational concepts in materials informatics and cheminformatics emphasizing quantitative structure property relationships QSPR The volume then presents various methods and tools including advanced QSPR models quantitative read across structure property relationship q RASPR models optimization strategies with minimal data and in silico studies using different descriptors Additionally it explores machine learning algorithms and their applications in materials science alongside innovative modeling approaches for quantum theoretic properties Overall the book serves as a comprehensive resource for understanding and applying machine learning in the study and development of advanced materials and is a useful tool for students researchers and professionals working in these areas

Multiscale Molecular Methods in Applied Chemistry Barbara Kirchner, Jadran Vrabec, 2012-01-25 First Principles Based Multiscale Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes by A Jaramillo Botero R Nielsen R Abrol J Su T Pascal J Mueller and W A Goddard Dynamic QM MM A Hybrid Approach to Simulating Gas Liquid Interactions by S Yockel and G C Schatz Multiscale Modelling in Computational Heterogeneous Catalysis by F J Keil Real World Predictions from Ab Initio Molecular Dynamics Simulations by B Kirchner P J di Dio and J Hutter Nanoscale Wetting Under Electric Field from Molecular Simulations by C D Daub D Bratko and A Luzar Molecular Simulations of Retention in Chromatographic Systems Use of Biased Monte Carlo Techniques to Access Multiple Time and Length Scales by J L Rafferty J I Siepmann M R Schure Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields by G Guevara Carrion H Hasse and J Vrabec Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes by L Delle Site C Holm and N F A van der Vegt Coarse Grained Modeling for Macromolecular Chemistry by H A Karimi Varzaneh and F M Iler Plathe

Journal American Chemical Society, 2004

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