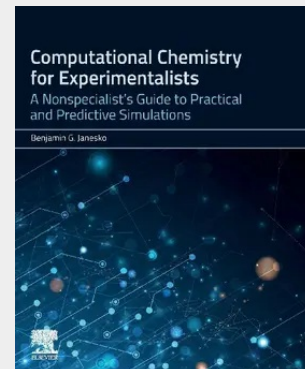


Computational Chemistry for Experimentalists

A Nonspecialist's Guide to Practical and Predictive Simulations

Computational Chemistry for Experimentalists: A Nonspecialist's Guide to Practical and Predictive Simulations empowers chemists--especially those at emerging institutions or in small and medium enterprises--by transforming foundational chemical concepts into practical computational skills. A modular approach, paired with hands-on video tutorials, ensures that even nonspecialists can confidently apply simulations to their research, regardless of career stage or specialization. Beyond its accessible structure, the book features six modules covering core topics such as electronic structure theory and molecular dynamics. Ten experimental modules focus on simulating specific laboratory techniques--reaction mechanisms, NMR, UV/vis, band structures, XPS, and organometallic chemistry. Regularly updated online tutorials complement the material, providing project-based, real-world training. By bridging theory and practice, this guide serves mid-career professionals, undergraduate and graduate students, and early-career researchers, making computational chemistry approachable and practical for all experimental chemists.



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