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Foundational Methods Enabling Science in an Integrated Ecosystem --Computational Workflow for Accelerated Molecular Design Using Quantum Chemical Simulations and Deep Learning Models -- Selflearning Data Foundation for Scientific AI -- Preconditioners for

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Sommario/riassunto

This book constitutes the refereed proceedings of the 22nd Smoky Mountains Computational Sciences and Engineering Conference on Accelerating Science and Engineering Discoveries Through Integrated Research Infrastructure for Experiment, Big Data, Modeling and Simulation, SMC 2022, held virtually, during August 23–25, 2022. The 24 full papers included in this book were carefully reviewed and selected from 74 submissions. They were organized in topical sections as follows: foundational methods enabling science in an integrated ecosystem; science and engineering applications requiring and motivating an integrated ecosystem; systems and software advances enabling an integrated science and engineering ecosystem; deploying advanced technologies for an integrated science and engineering ecosystem; and scientific data challenges.