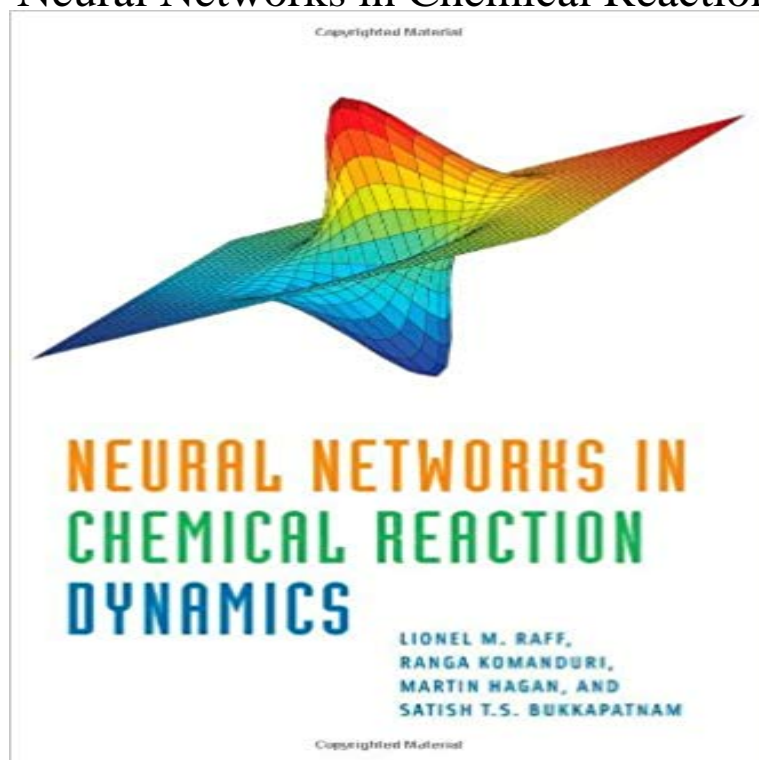


# Neural Networks in Chemical Reaction Dynamics



This monograph presents recent advances in neural network (NN) approaches and applications to chemical reaction dynamics. Topics covered include: (i) the development of ab initio potential-energy surfaces (PES) for complex multichannel systems using modified novelty sampling and feedforward NNs; (ii) methods for sampling the configuration space of critical importance, such as trajectory and novelty sampling methods and gradient fitting methods; (iii) parametrization of interatomic potential functions using a genetic algorithm accelerated with a NN; (iv) parametrization of analytic interatomic potential functions using NNs; (v) self-starting methods for obtaining analytic PES from ab initio electronic structure calculations using direct dynamics; (vi) development of a novel method, namely, combined function derivative approximation (CFDA) for simultaneous fitting of a PES and its corresponding force fields using feedforward neural networks; (vii) development of generalized PES using many-body expansions, NNs, and moiety energy approximations; (viii) NN methods for data analysis, reaction probabilities, and statistical error reduction in chemical reaction dynamics; (ix) accurate prediction of higher-level electronic structure energies (e.g. MP4 or higher) for large databases using NNs, lower-level (Hartree-Fock) energies, and small subsets of the higher-energy database; and finally (x) illustrative examples of NN applications to chemical reaction dynamics of increasing complexity starting from simple near equilibrium structures (vibrational state studies) to more complex non-adiabatic reactions. The monograph is prepared by an interdisciplinary group of researchers working as a team for nearly two decades at Oklahoma State University, Stillwater, OK with expertise in gas phase reaction dynamics; neural networks; various aspects of MD and Monte Carlo (MC) simulations

of nanometric cutting, tribology, and material properties at nanoscale; scaling laws from atomistic to continuum; and neural networks applications to chemical reaction dynamics. It is anticipated that this emerging field of NN in chemical reaction dynamics will play an increasingly important role in MD, MC, and quantum mechanical studies in the years to come.

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