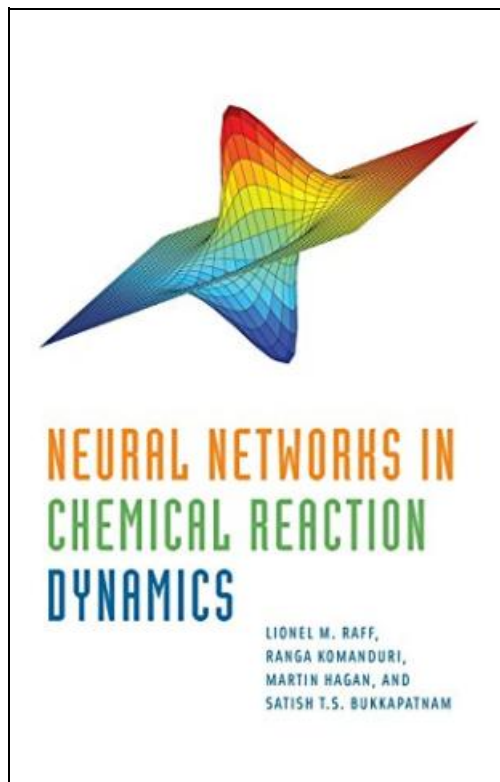# Neural Networks in Chemical Reaction Dynamics

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(Dr. Torrey Osinski DVM)

NEURAL NETWORKS IN CHEMICAL REACTION DYNAMICS

Oxford University Press. Hardcover. Condition: New. 312 pages. Dimensions: 9.3in. x 6.3in. x 1.0in.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 inito 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...

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