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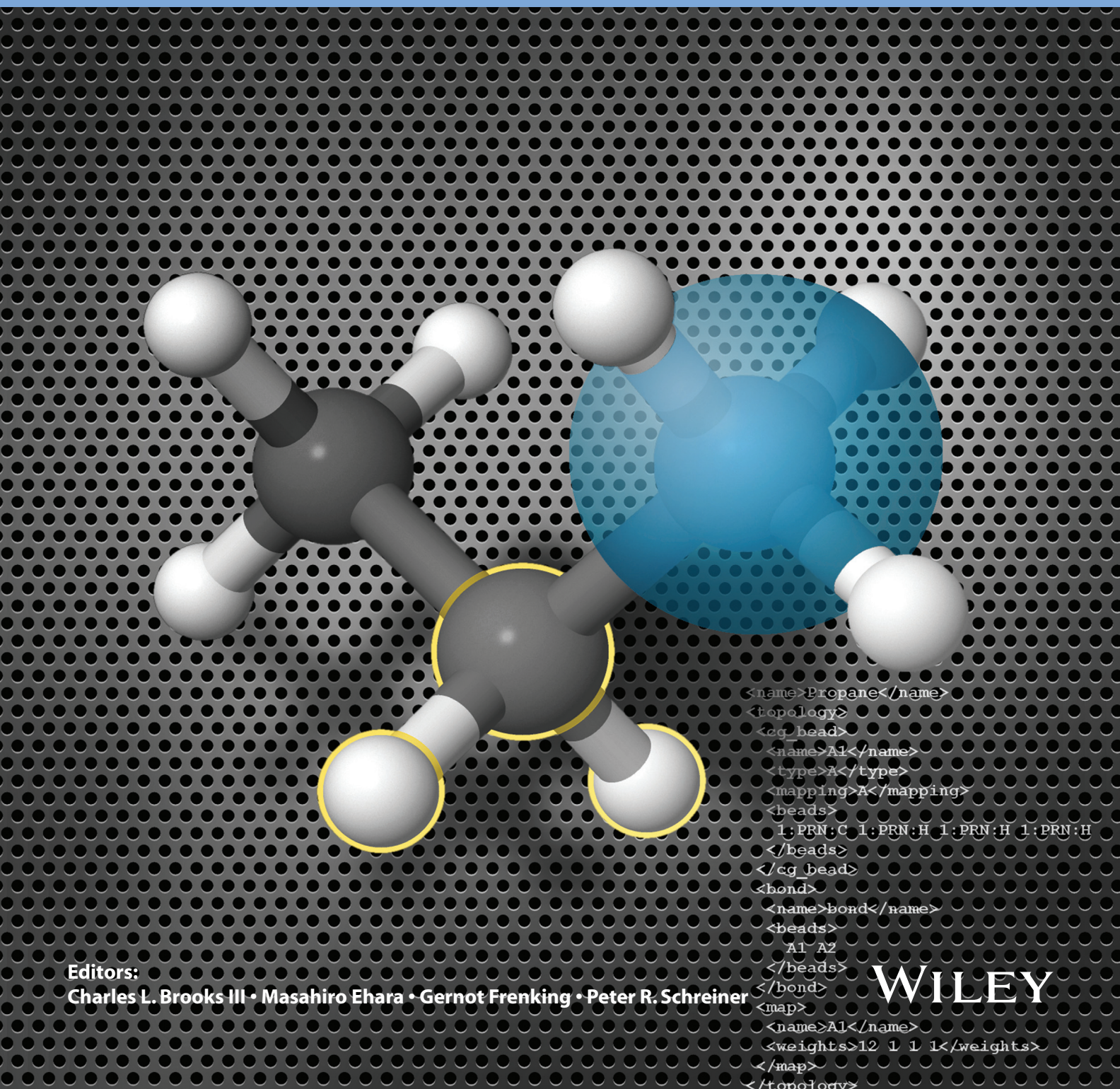

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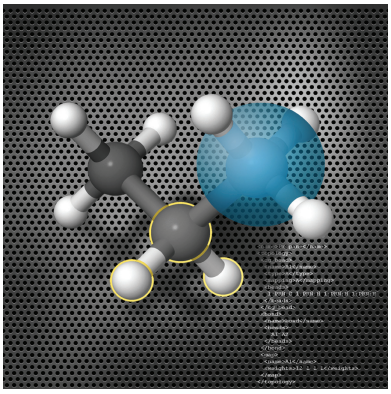
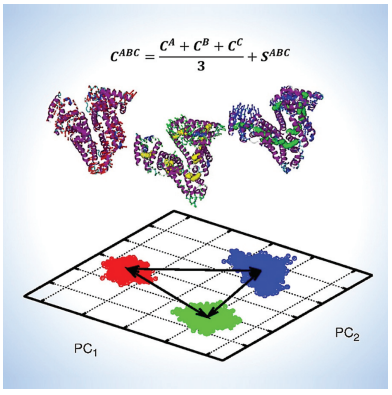


Structure Mapping

On page 467, Staš Bevc, Christoph Junghans, and Matej Praprotnik report on STOCK (structure mapper and Online Coarse-graining Kit), a web toolkit available at http://stock.cmm.ki.si that aids users in setting up coarse-grained molecular simulations. The toolkit includes a structure mapper to visually define a molecular mapping from fine- to coarse-grained models and a web-based implementation of the Boltzmann inversion method to derive effective potentials between coarse-grained beads. The cover shows the building up of a coarse-grained model of the propane molecule using STOCK. The blue sphere is a coarse-grained bead, mapped to four atoms. Atoms surrounded by yellow circles are selected to be mapped to a bead. Text at the bottom right defines the mapping and is automatically generated by STOCK.



Principal Component Analysis

Combined principal component analysis (combined-PCA) is a technique usually employed to analyze structural and dynamical differences between alternative conformations of a given protein. However, analytical formulas showing what is and is not to be expected from a combined-PCA have never been provided. On page 424, Gustavo Pierdominici-Sottile and Juliana Palma present and discuss such formulas, which can guide the development of combined-PCA. The final expressions can be summarized as follows: the correlation matrix of a concatenated trajectory is given by the average of the individual correlation matrices plus the correlation matrix of the individual average structures.

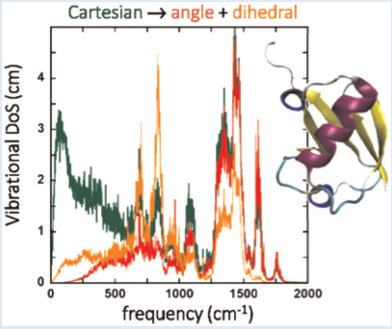
Coming Soon

Look for these important papers in upcoming issues

Internal Coordinate Density of State from Molecular Dynamics Simulation

Shiang-Tai Lin et al.

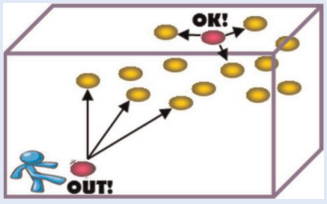
The Wilson's **B**-matrix method is generalized to calculate the internal coordinate density of state (DoS) of macromolecules. Compared with the Cartesian DoS where the normal modes are a superposition of various internal modes, the internal DoS allows a clear association of each vibrational mode with the dynamic behavior of a system, and thus provides a more natural way to describe molecular motion.
DOI: 10.1002/jcc.23822



k-Nearest Neighbors Optimization-Based Outlier Removal

Hanoch Senderowitz et al.

A new iterative method for the identification and removal of outliers from quantitative structure activity relationship (QSAR) datasets is described. This method is based on a *k*NN optimization algorithm, and is named *k*NN optimization-based outlier removal. It can maintain the internal diversity of the parent dataset while producing QSAR models with better prediction statistics than other outlier removal methods.
DOI: 10.1002/jcc.23803



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