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Materials Dynamics Descriptors Determined by MD Data. SVEN RUDIN, Los Alamos National Laboratory — How do we choose descriptors for the dynamic behavior of a material? An information science-based possibility builds upon an approach to analyze the atomic movement in a material simulated with molecular dynamics [Physical Review B 97, 134114 (2018)]. By sampling the correlated atomic movement, a set of collective vibrational modes are defined that show no correlation between them. These "Principal Vibrational Modes" (PVMs) represent a transparent framework to understand and describe a material's nonlinear dynamical properties. The mode with the largest amplitude, e.g., emerges as a natural descriptor indicating the structural phase. The PVMs constitute a list of dynamics descriptors that is ordered according to the modes' amplitudes. Collective atomic movement with large amplitudes generally correlates with important materials behavior and properties. This suggests the PVMs can serve as dynamics descriptors of materials.

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