STANFORD
UNIVERSITY

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February 26, 2016

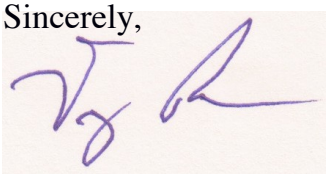
Dear Dr. Lester,

We are submitting the following report, entitled "Identification of simple reaction coordinates from complex dynamics," for publication in the *Journal of Chemical Physics*.

The subject of this manuscript is the inference of reaction coordinates from molecular dynamics (MD) simulations. We first introduce a general definition of the reaction coordinate suitable for condensed phase and biomolecular systems, which we show is equivalent to a leading eigenfunction of an integral operator governing a system's ensemble dynamics. Subsequently, we develop a practical new estimator designed to find sparse, interpretable approximations to these reaction coordinates from MD simulations using a small number of structural order parameters. This work bridges recent developments in the fields of machine learning and optimization, such as sparsity-inducing regularizers and the alternating direction method of multipliers, with contemporary needs in biological and chemical physics arising out of the analysis of large-scale simulation data sets. We anticipate this report will be of interest to the broad readership of *JCP*.

Below, we provide a list of potential reviewers.

Sincerely,



Vijay Pande
Camille and Henry Dreyfus Distinguished Chair in Chemistry and (by courtesy)
Professor of Structural Biology and of Computer Science
Director, Program in Biophysics
Director, Folding@home Distributed Computing Project

List of suggested reviewers:

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