

Problem set 6: Computational Molecular Physics

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(Please send the solution by e-mail to tahereh.ghane@gmail.com by **Thu. 11.06 (4pm)** at the latest.)

1 PCCA

(40 points) Choose your favorite programming language and do a metastability analysis of the transition matrix T_{mat} according to this exercise :

- (a) Calculate the eigenvalues of the matrix and plot them.
- (b) Based on part(a) decide how many eigenvectors you want to look at and plot these eigenvectors in such a way that you can determine the simplex structure for PCCA.
- (c) Find the transformation matrix using information of part (b).
- (d) Define the characteristic vectors and plot them and discuss the result of this part.