

Monday, April 24, 2017

POSTER SESSION I:

ORIGIN AND EVOLUTION OF LIFE: PREBIOTIC BIOCHEMISTRY:

AB INITIO COMPUTATIONAL PREBIOTIC CHEMISTRY

7:00 p.m. Main Hall

Kroonblawd M. P. Goldman N.

[Improving Density Functional Tight Binding Predictions of Free Energy Surfaces for Peptide Condensation Reactions in Solution](#) [#3303]

A force matching approach is presented to increase the accuracy of semi-empirical (DFTB) free energy surface predictions for slow reactions.