Enhanced Sampling Techniques

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Chapter 1

Introduction

Method	T_{max}K	λ	ϵ_{CA}	κ	ϵ_{OW}
–	300	1.0	0.359824	1.0	0.998989
REST2	450	0.666667	0.239883	1.0	0.998989
ssREST3	450	0.666667	0.239883	1.1	1.20878

Table 1.1: Table showing the differences and similarities of ϵ scaling between the REST2 and ssREST3 methods. In case of ssREST3 the water ϵ gets scaled along with the solute ϵ by a factor if κ^2 where as solvent parameters are not scaled during REST2.