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镎(IV)、镅(III)、锔(III)的 Amber 力场参数化及评估

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Parameterization and Validation of Amber Force Field for Np^{4+}, Am^{3+}, and Cm^{3+}

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1 RDF

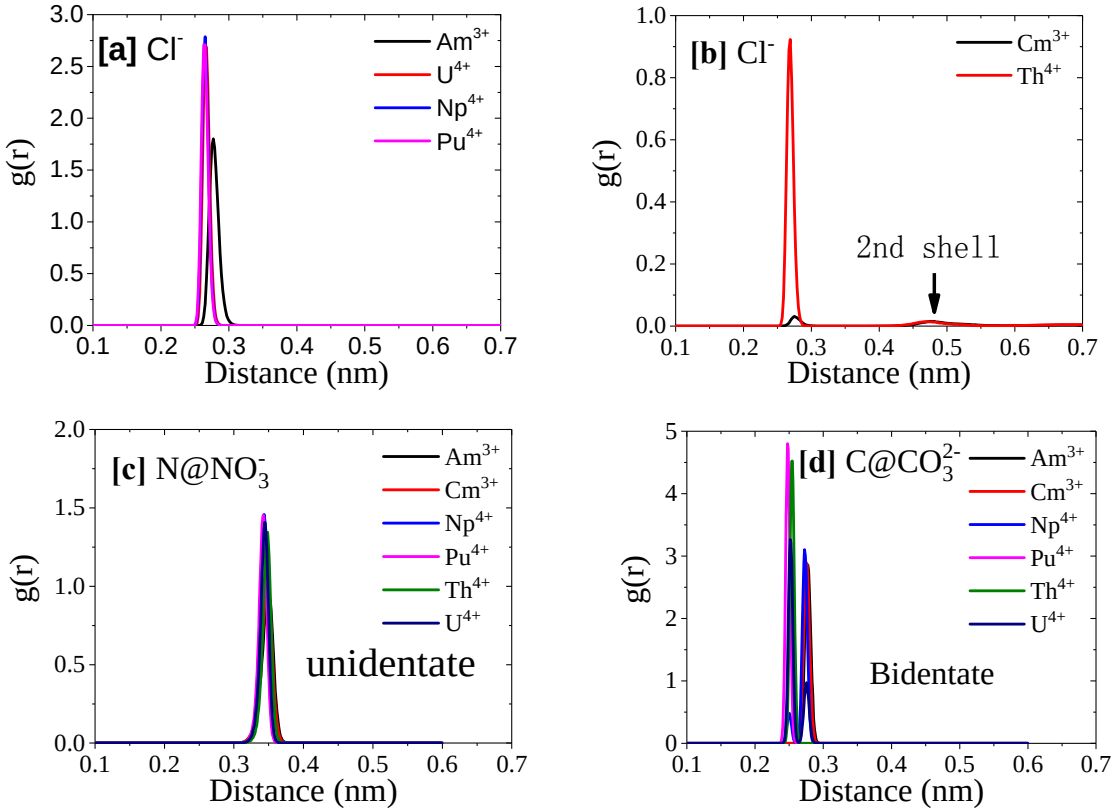

图 S1　在 20 ns 模拟中 $An^{3+/4+}$周围 Cl^-、NO_3^-的 N 原子、CO_3^{2-}的 C 原子的 RDF 统计

Fig. S1　The RDF of Cl^-, N atom of NO_3^-, C atom of CO_3^{2-} around $An^{3+/4+}$ in 20 ns sampling simulations.

2 Free energy integral

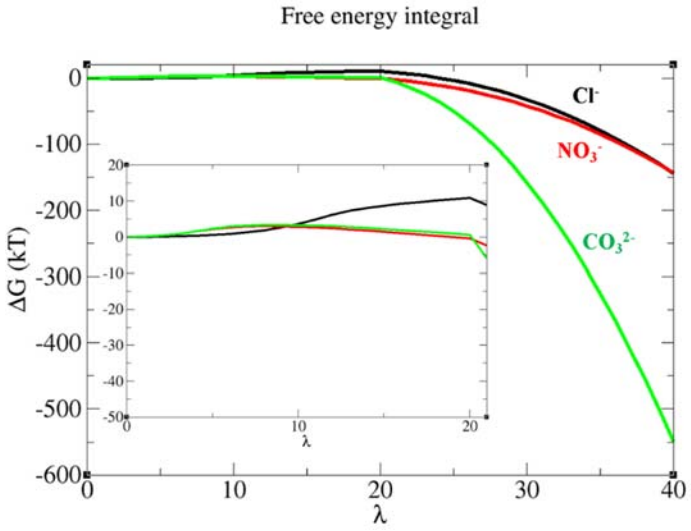

图 S2　Cl^-、NO_3^-及 CO_3^{2-}的水合自由能微扰过程中窗口序号从 0–40 时的自由能数值积分

Fig. S2　The free energy integral from window number 0–40 in the FEP calculations of Cl^-, NO_3^-, and CO_3^{2-}.

The window number 0–20 represents the perturbation of vdW interaction, while 21–40 represents the perturbation of electrostatic interaction.

3 Correlation function of residence time

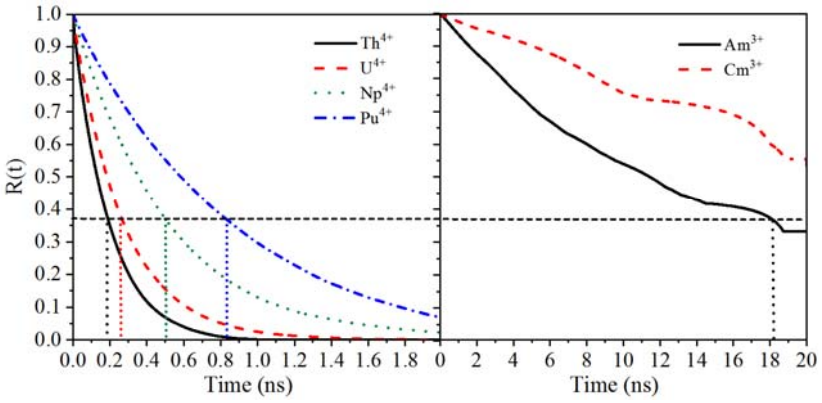

图 S3　四价锕系(Th^{4+}、U^{4+}、Np^{4+}、Pu^{4+}) (左图)和三价锕系(Am^{3+}、Cm^{3+}) (右图)第一配位层水分子的驻留时间的时间相关函数，及其驻留时间的取值

Fig. S3　The residence time of 1st coordination shell water during the 20 ns MD simulations for tetravalent cations (left, Th^{4+} in black, U^{4+} in red, Np^{4+} in green and Pu^{4+} in blue) and trivalent cations (right, Am^{3+} in black and Cm^{3+} in red).