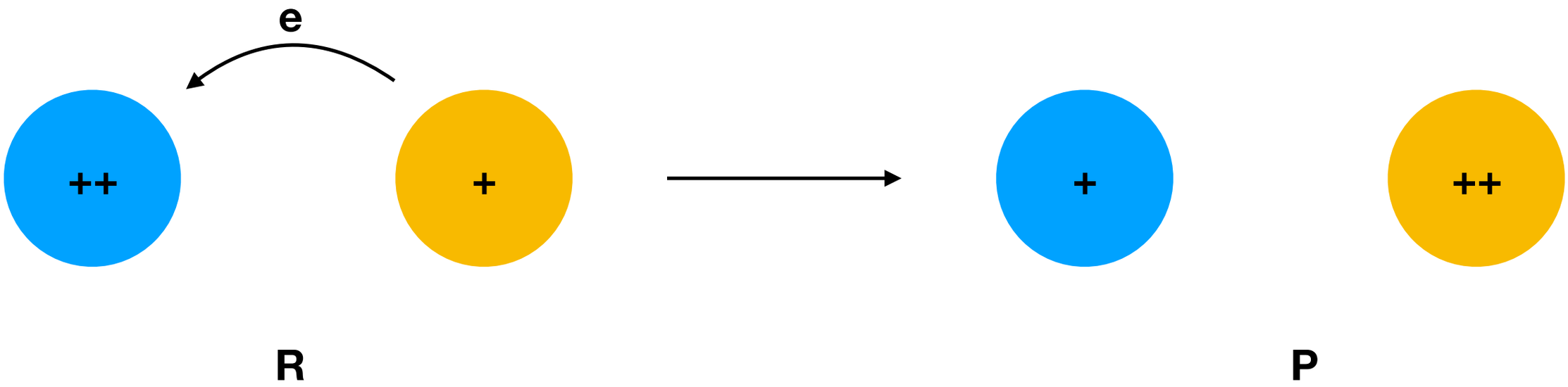
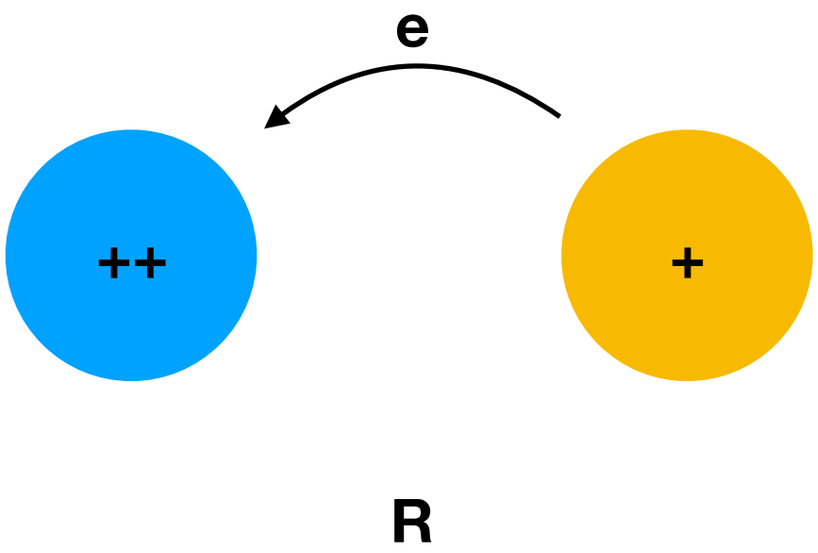
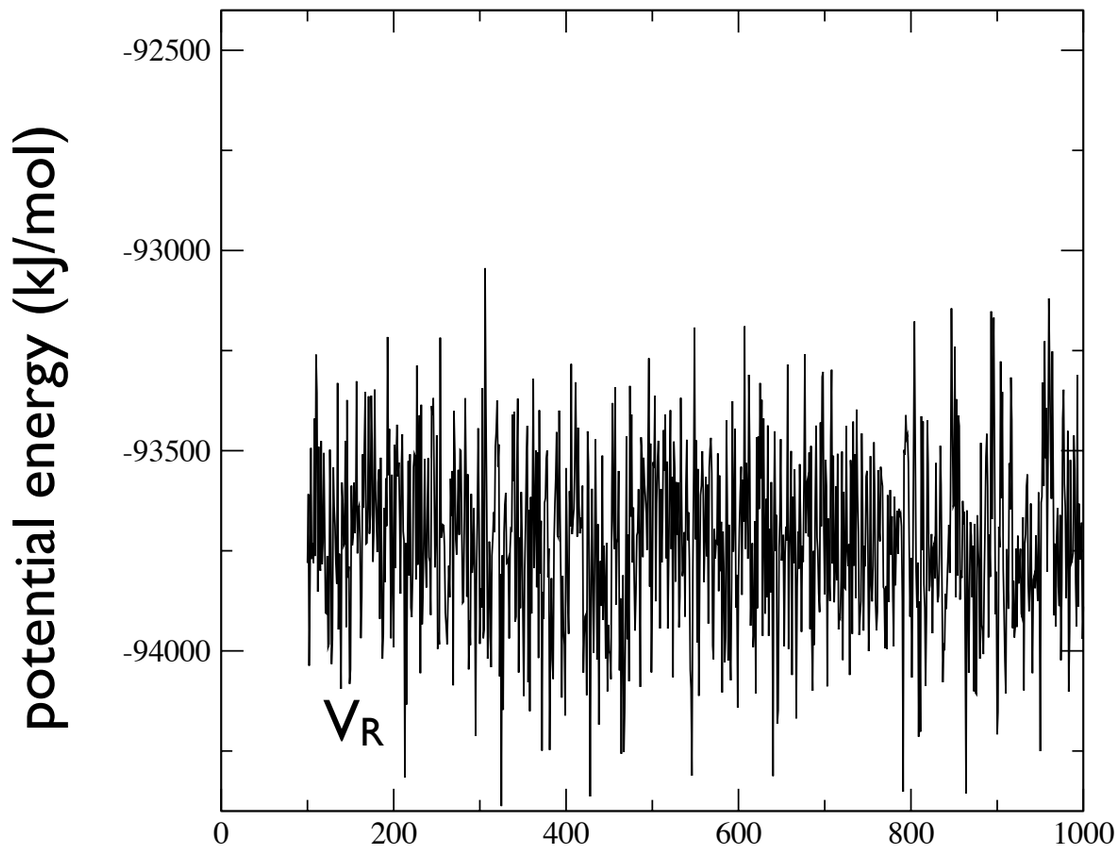
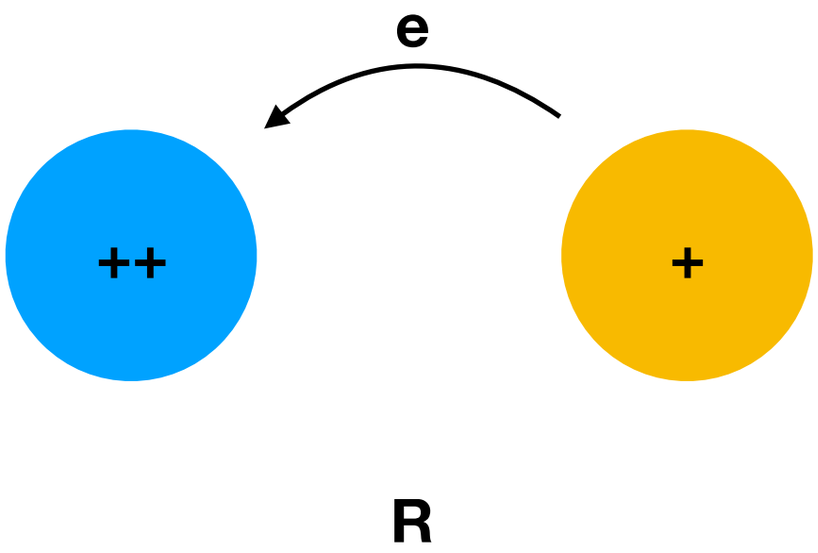

e
++
+
+
++
R
P



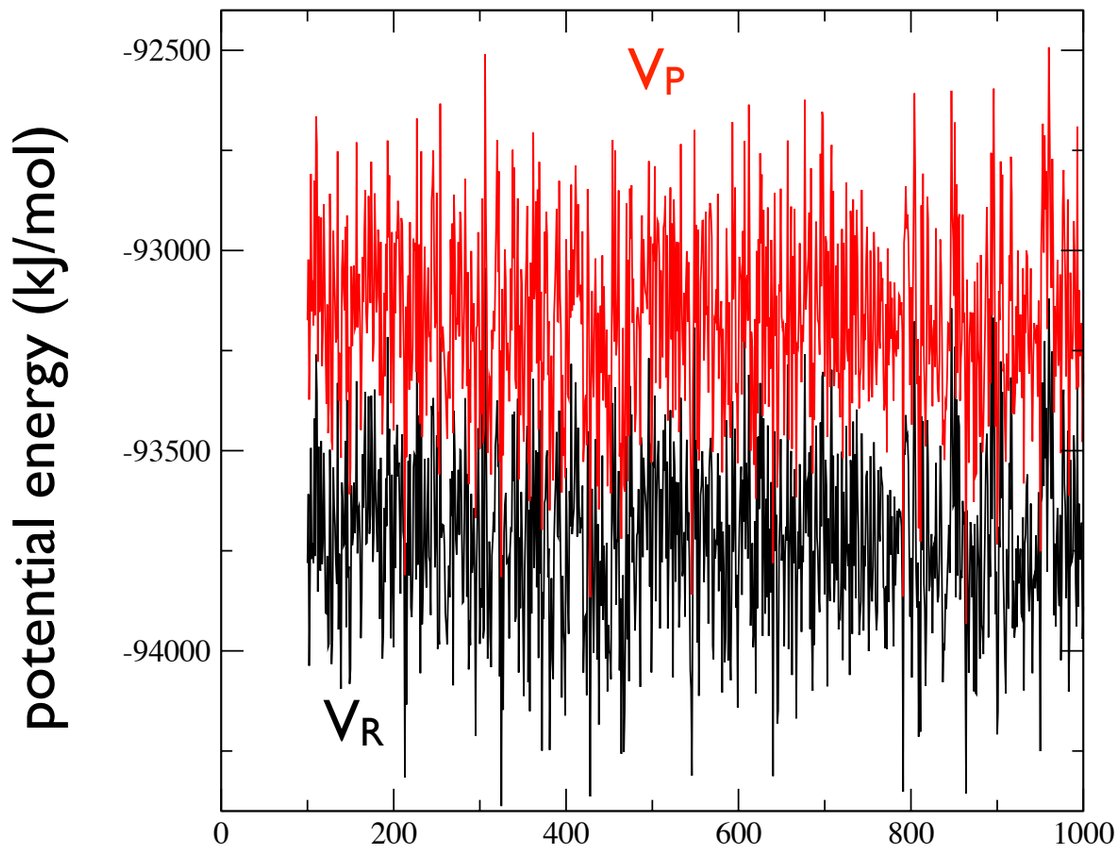
MC or MD simulation of R



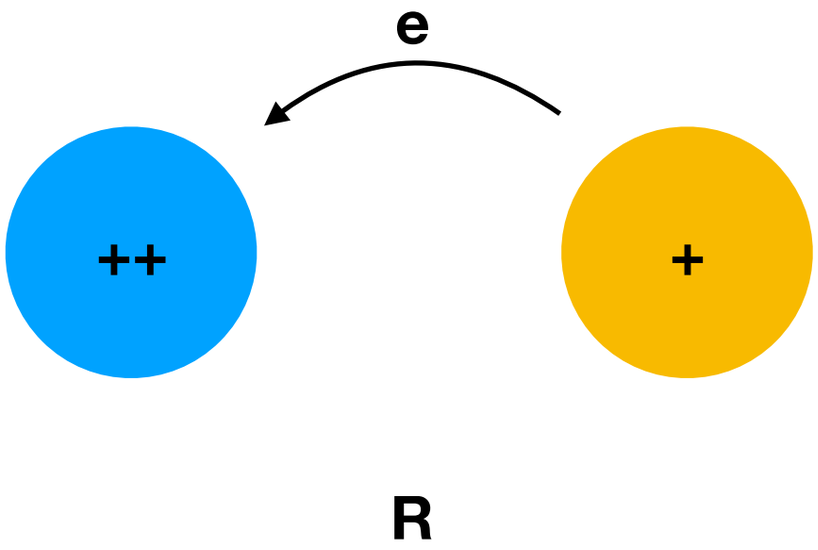
time (ps)



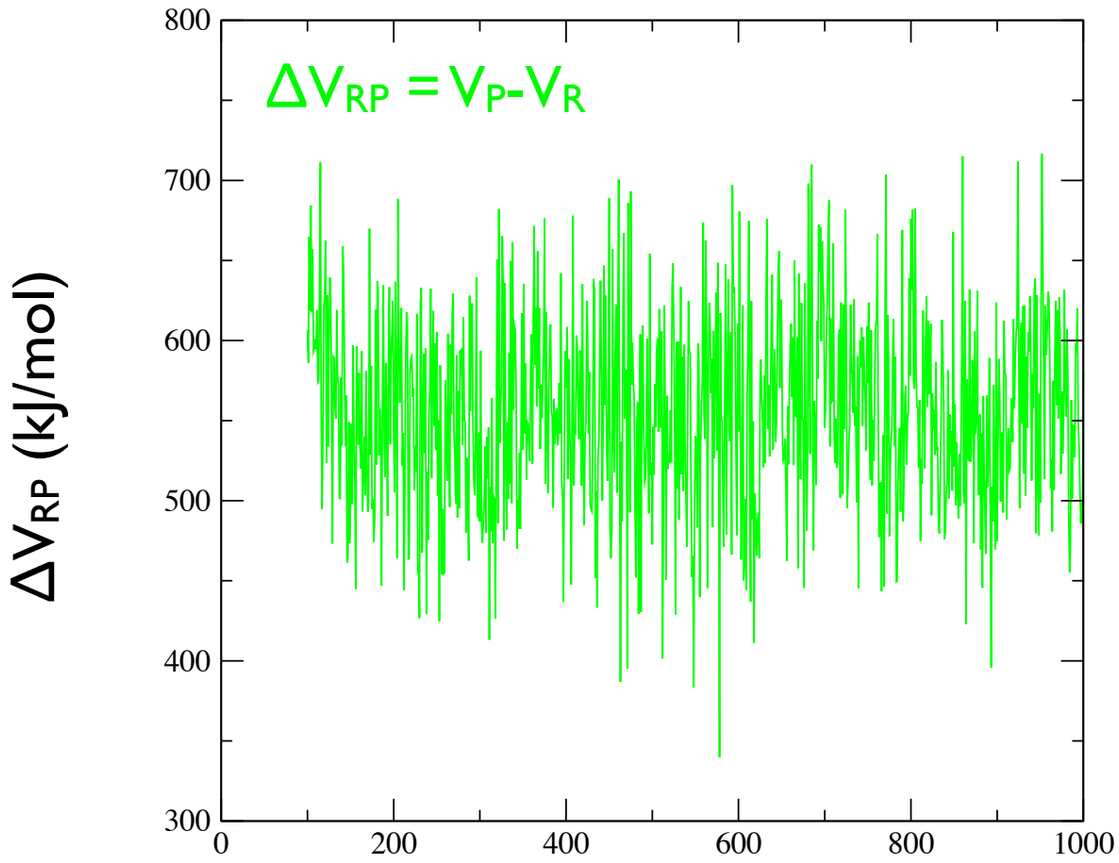
MC or MD simulation of R



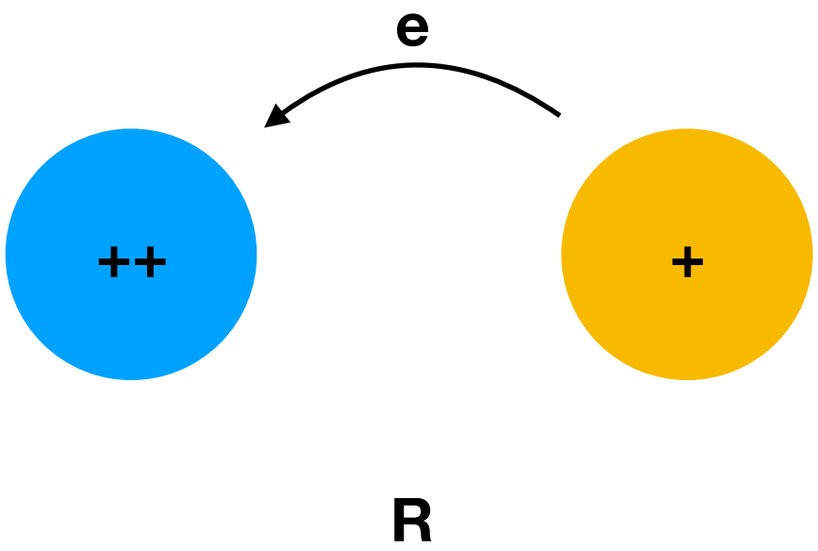
time (ps)



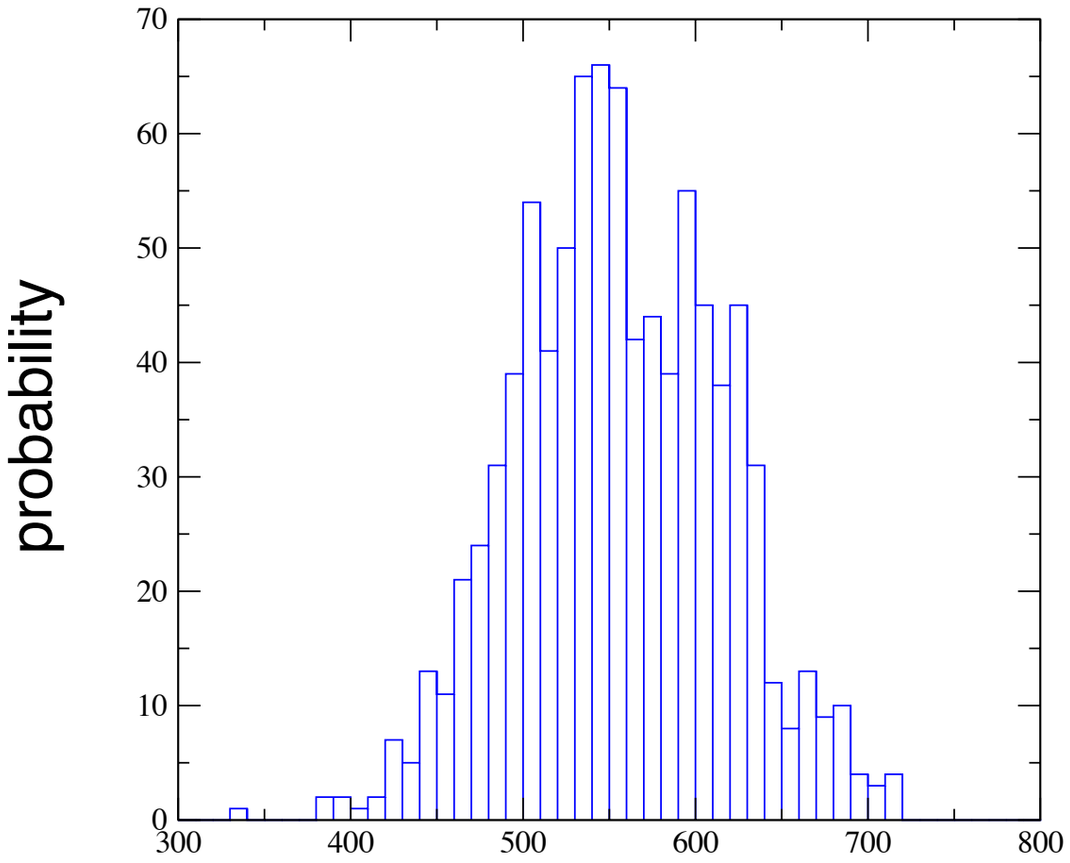
MC or MD simulation of R



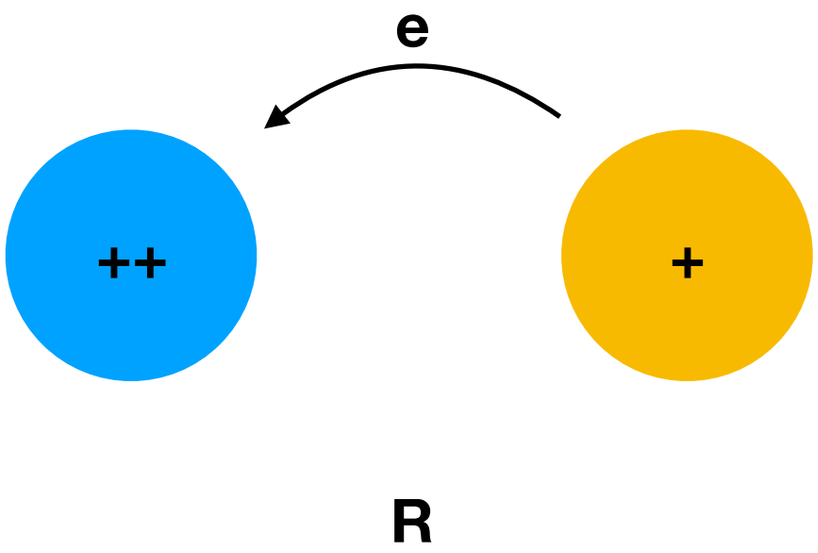
time (ps)



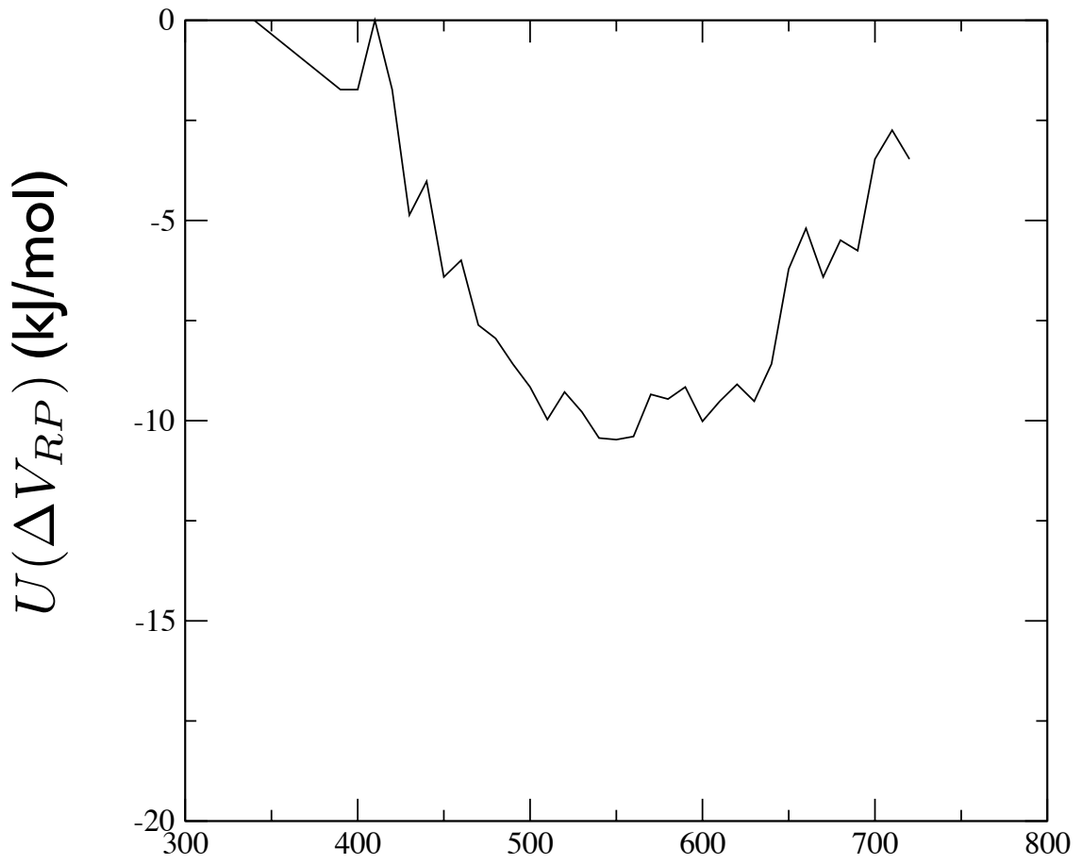
MC or MD simulation of R



$$p(\Delta V_{RP}) = \frac{1}{Z} e^{-\beta U(\Delta V_{RP})}$$



MC or MD simulation of R

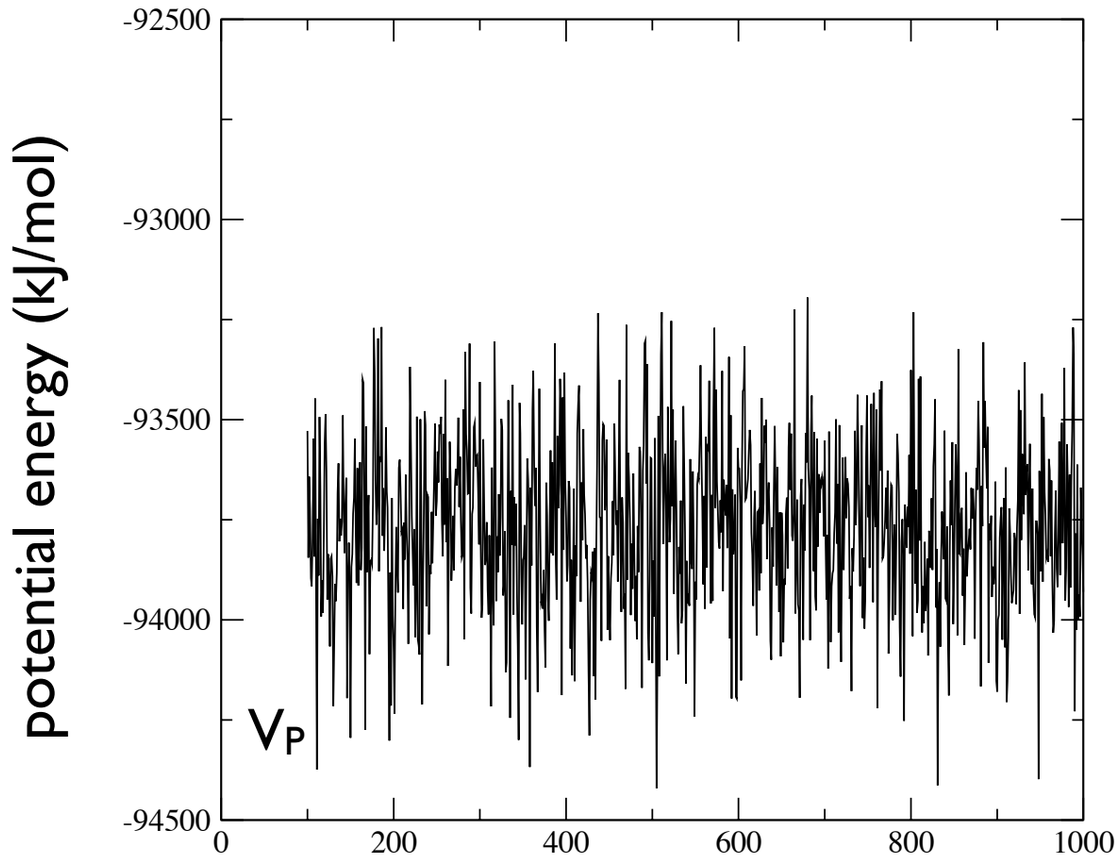


$$p(\Delta V_{RP}) = \frac{1}{Z} e^{-\beta U(\Delta V_{RP})}$$

$$U(\Delta V_{RP}) = -k_{\mathrm{B}} T \ln p(\Delta V_{RP}) - k_{\mathrm{B}} T \ln Z$$

P

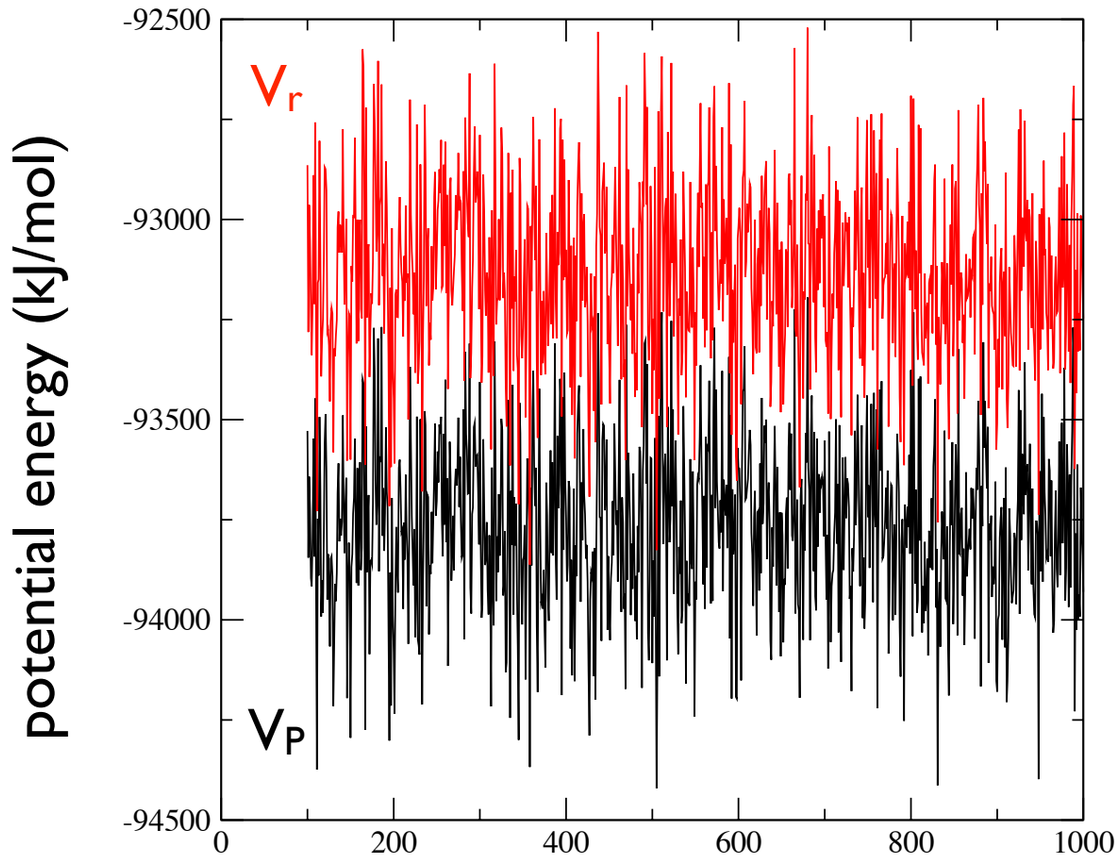
MC or MD simulation of P



time (ps)

P

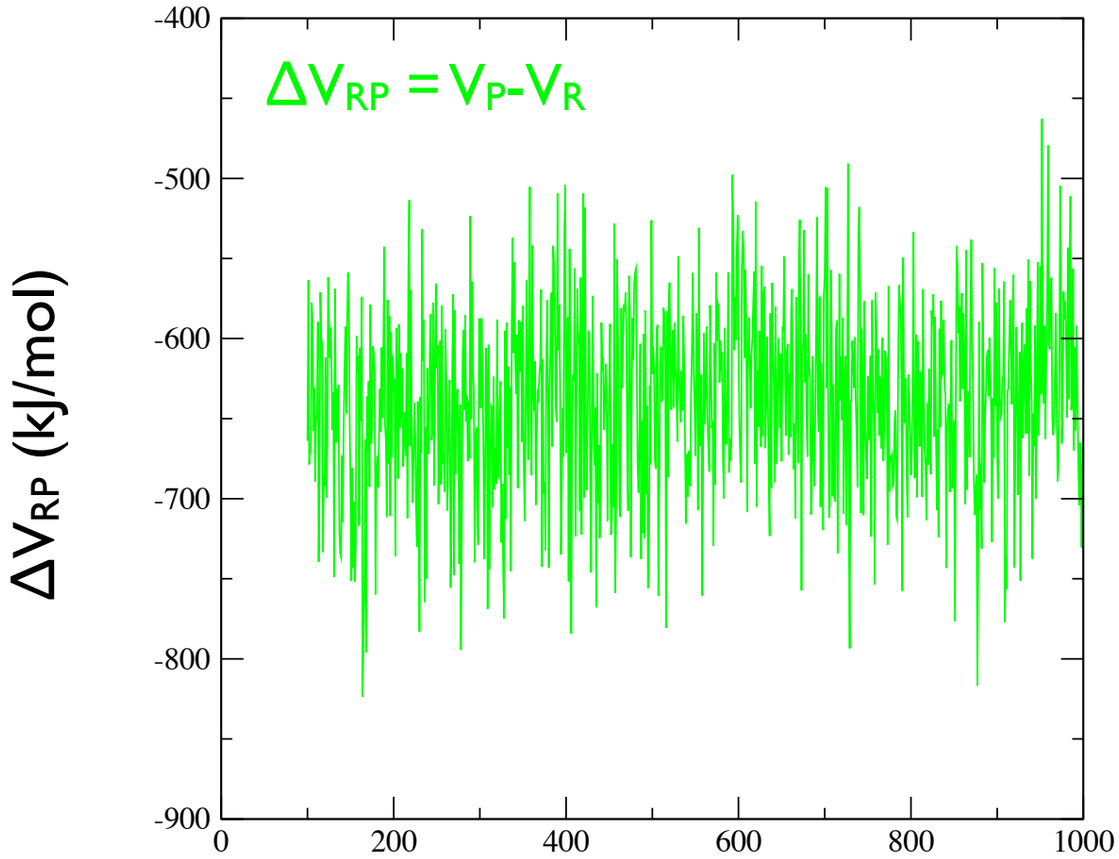
MC or MD simulation of P



time (ps)

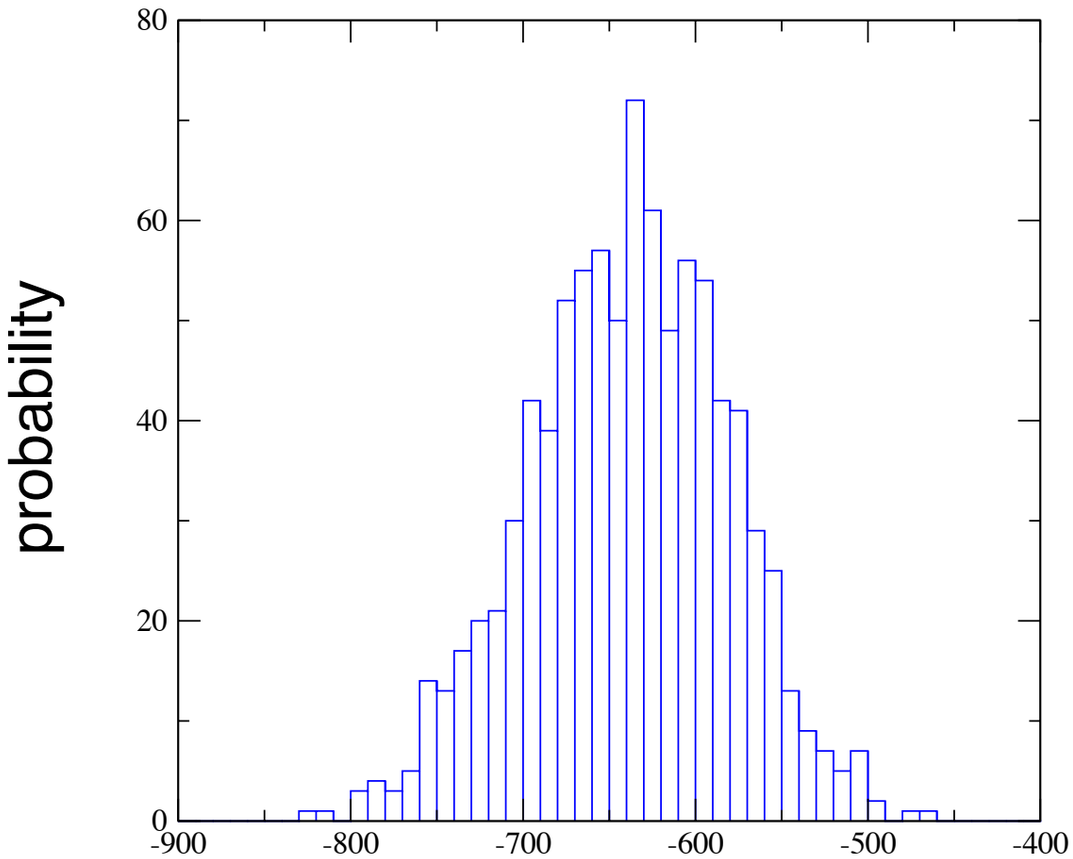
P

MC or MD simulation of P



P

MC or MD simulation of P

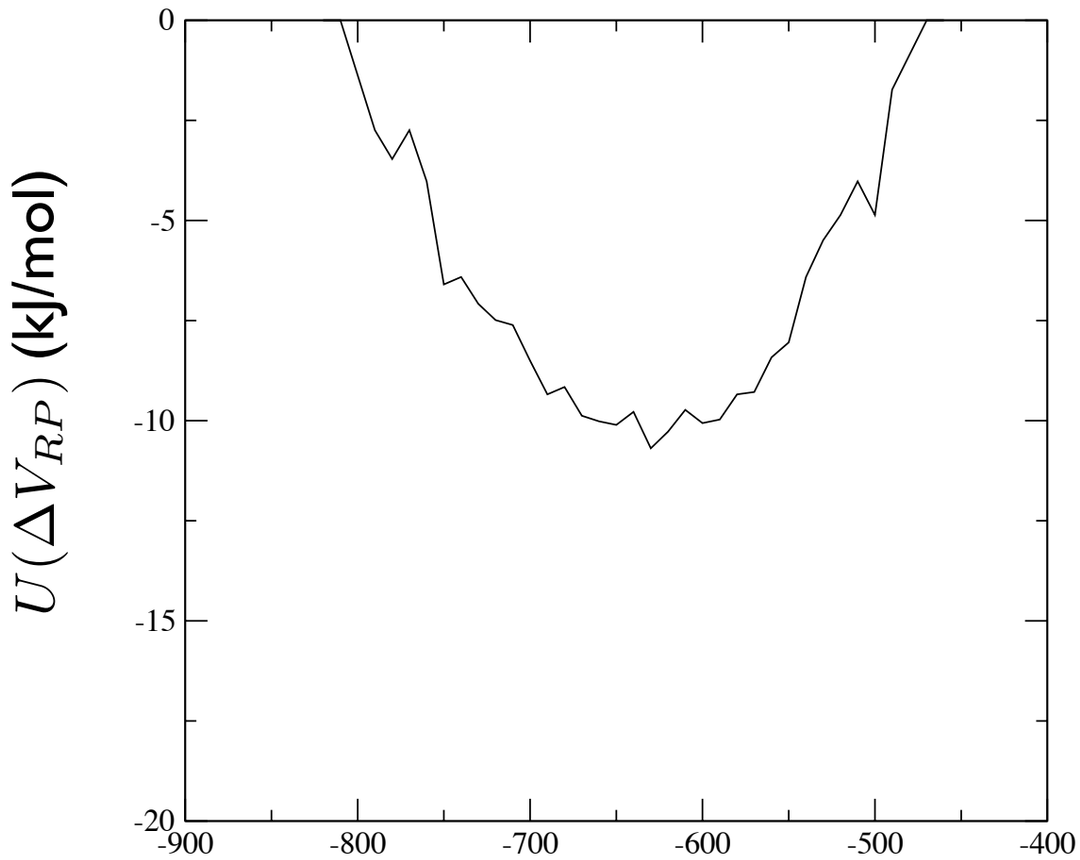


ΔV_{RP} (kJ/mol)

$$p(\Delta V_{RP}) = \frac{1}{Z} e^{-\beta U(\Delta V_{RP})}$$

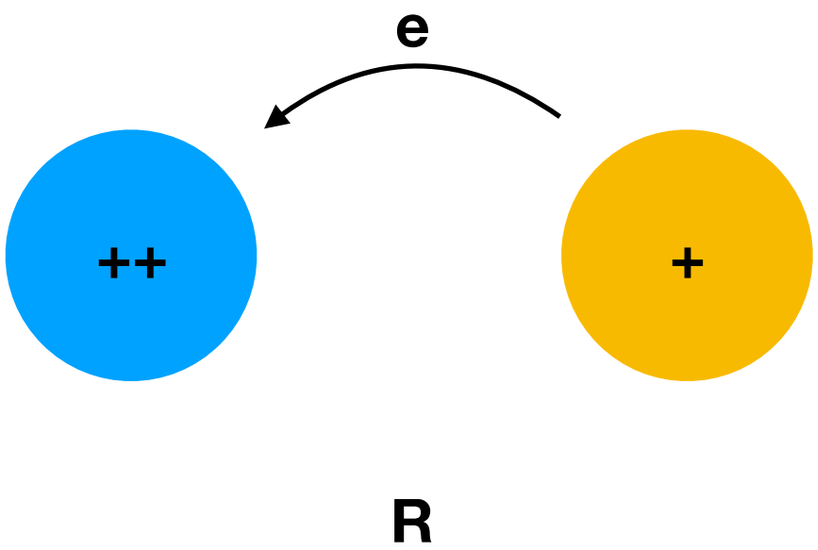
P

MC or MD simulation of P



$$p(\Delta V_{RP}) = \frac{1}{Z} e^{-\beta U(\Delta V_{RP})}$$

$$U(\Delta V_{RP}) = -k_{\mathrm{B}} T \ln p(\Delta V_{RP}) - k_{\mathrm{B}} T \ln Z$$



MC or MD simulation of R & P