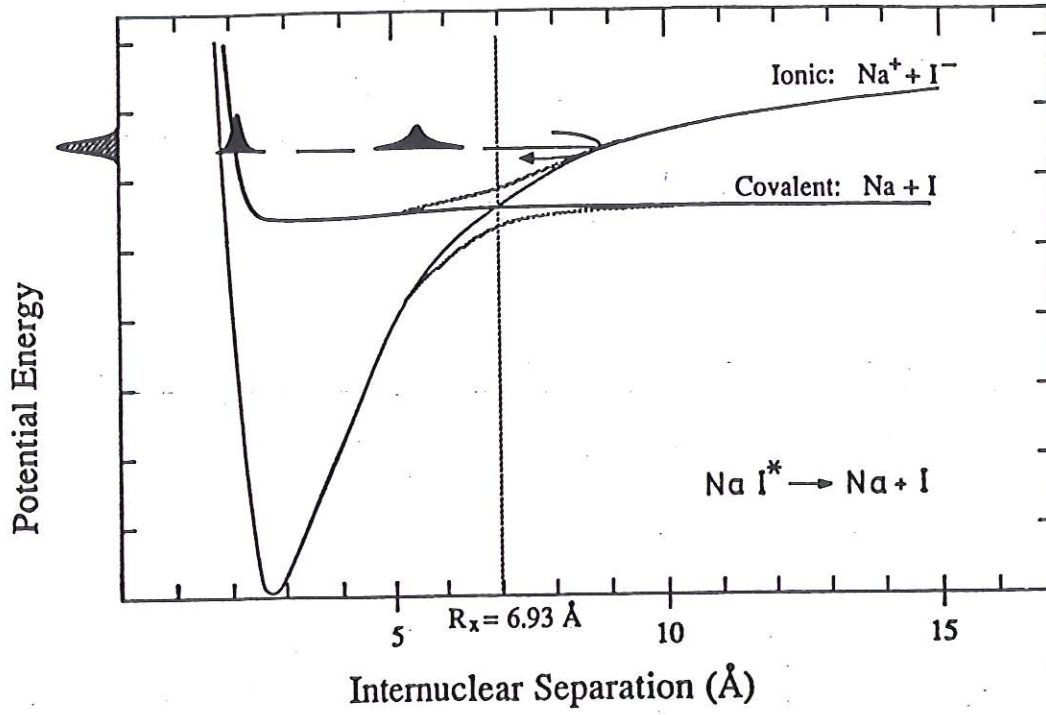
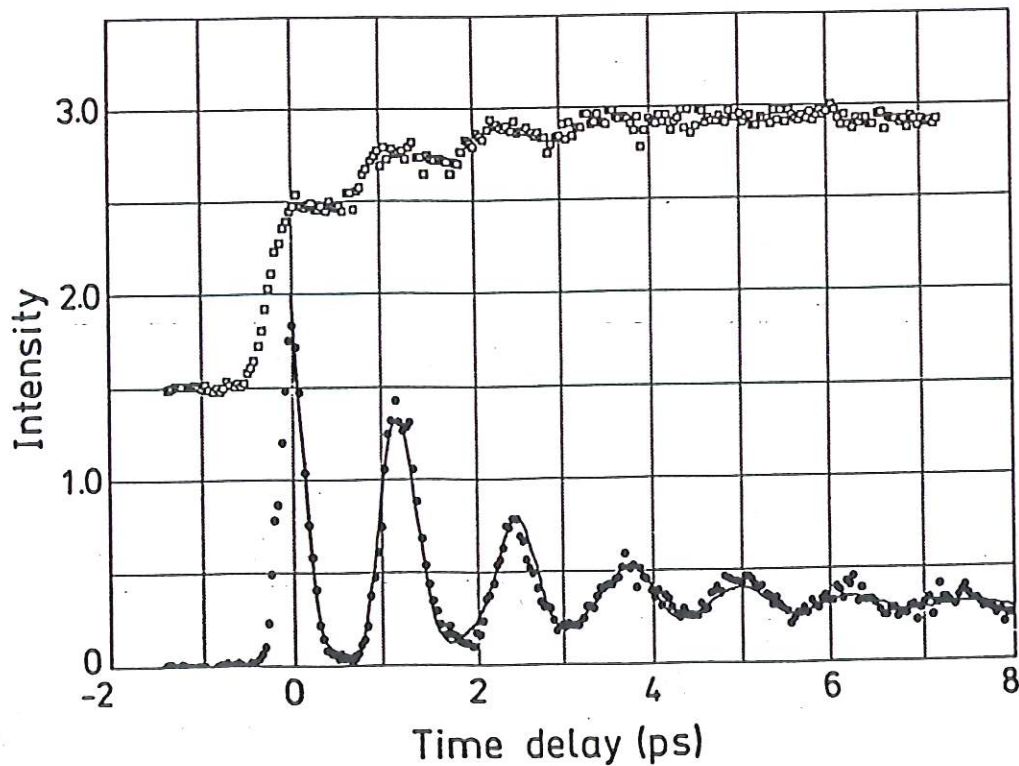


Photodissoziation von NaI



Zewail et al (1988)



CI-expansion for (weakly) avoided crossing

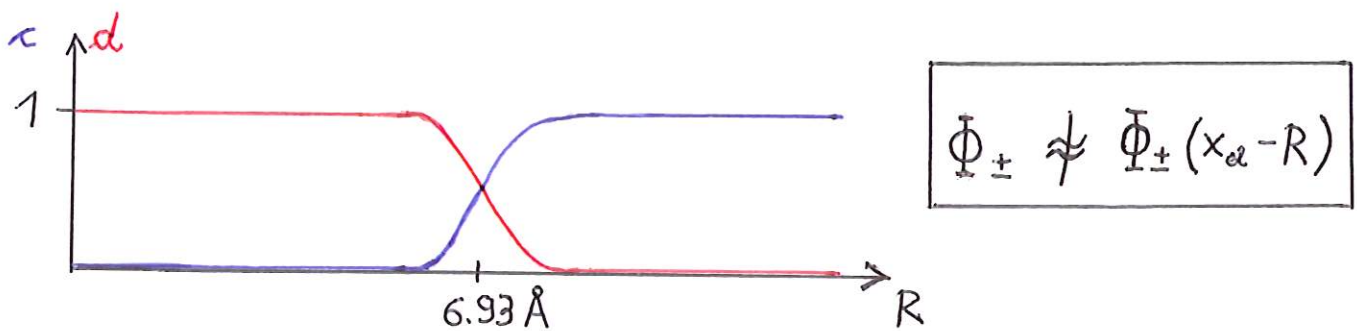
$$R < 6 \text{ \AA} \quad \Phi_1 \equiv \Phi_+ \approx \Phi_{\text{NaI}} = \Phi_{\text{cov}}$$

$$\Phi_0 \equiv \Phi_- \approx \Phi_{\text{Na}^+\text{I}^-} = \Phi_{\text{ion}}$$

$$R > 8 \text{ \AA} \quad \Phi_0 \equiv \Phi_- \approx \Phi_{\text{NaI}} = \Phi_{\text{cov}}$$

$$\Phi_1 \equiv \Phi_+ \approx \Phi_{\text{Na}^+\text{I}^-} = \Phi_{\text{ion}}$$

General: $\Phi_0 = c \Phi_{\text{cov}} + d \Phi_{\text{ion}}$



Φ_{cov} and Φ_{ion} are examples of diabatic electronic wave-functions (do not [always] diagonalize the electronic Hamiltonian).

Situation typical for alkali halides.

Situation generic to weakly avoided crossings.

Nonadiabatic coupling effects evident from experiment.