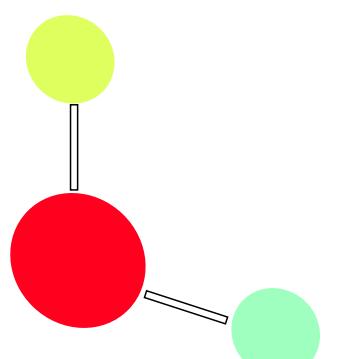


ADDITIONAL PROJECTS

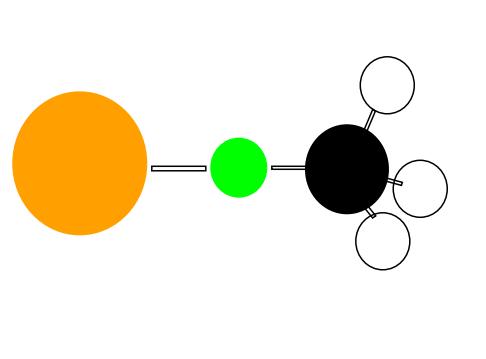
M. Oppel

ABC



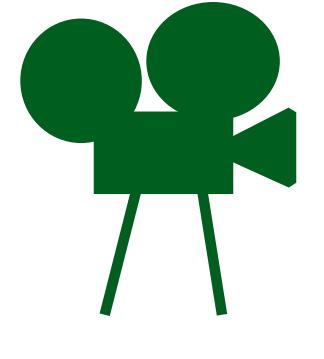
COOPERATIONS
TP A2 (Hertel/Korn)
G.K. Paramonov (Minsk)
M.V. Korolkov (Minsk)

BaFCH₃



COOPERATIONS
TP A4 (Radloff/Schulz)
H.-H. Ritze (MBI)
G.K. Paramonov (Minsk)
M.V. Korolkov (Minsk)

Simulation and Visualisation

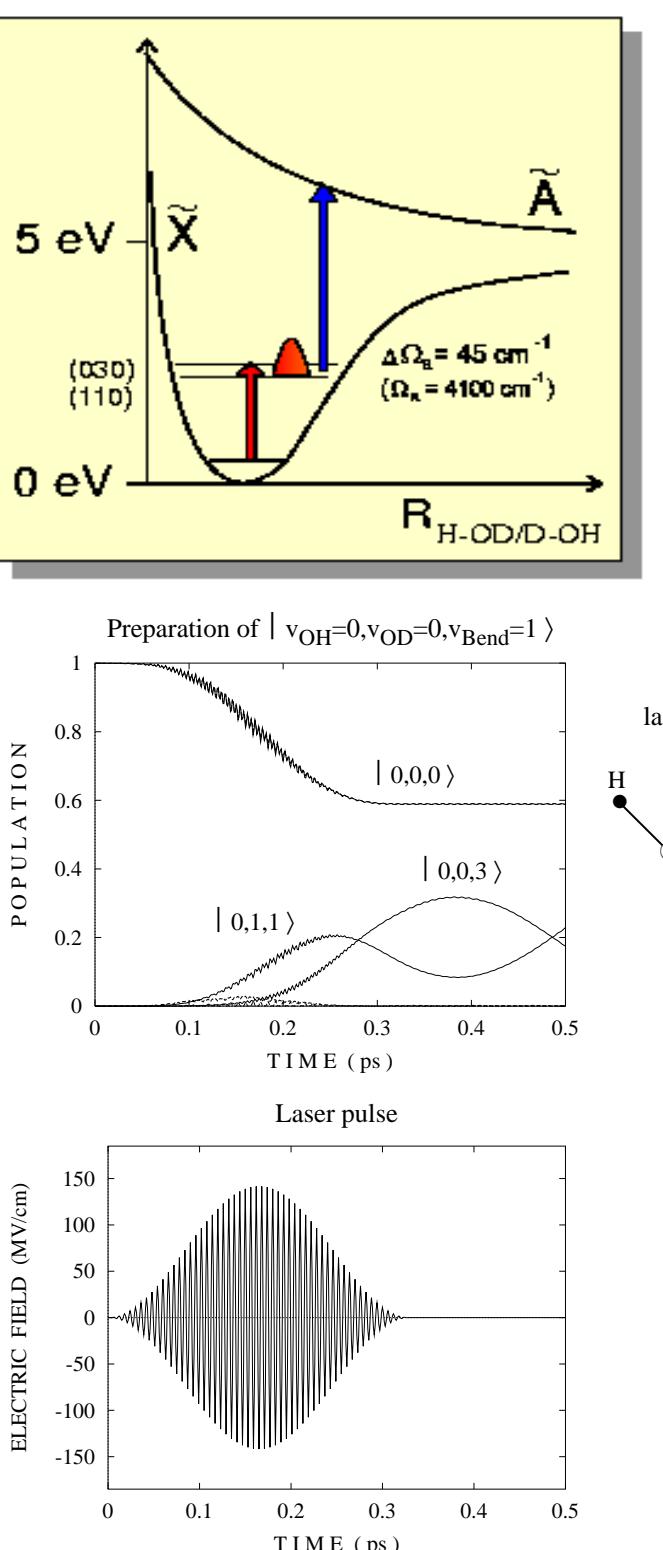


COWORKERS
M. Dahlmann
N. Elghobashi
P. Krause
Ch. Salzmann

RESULTS

HOD

IR+UV Excitation

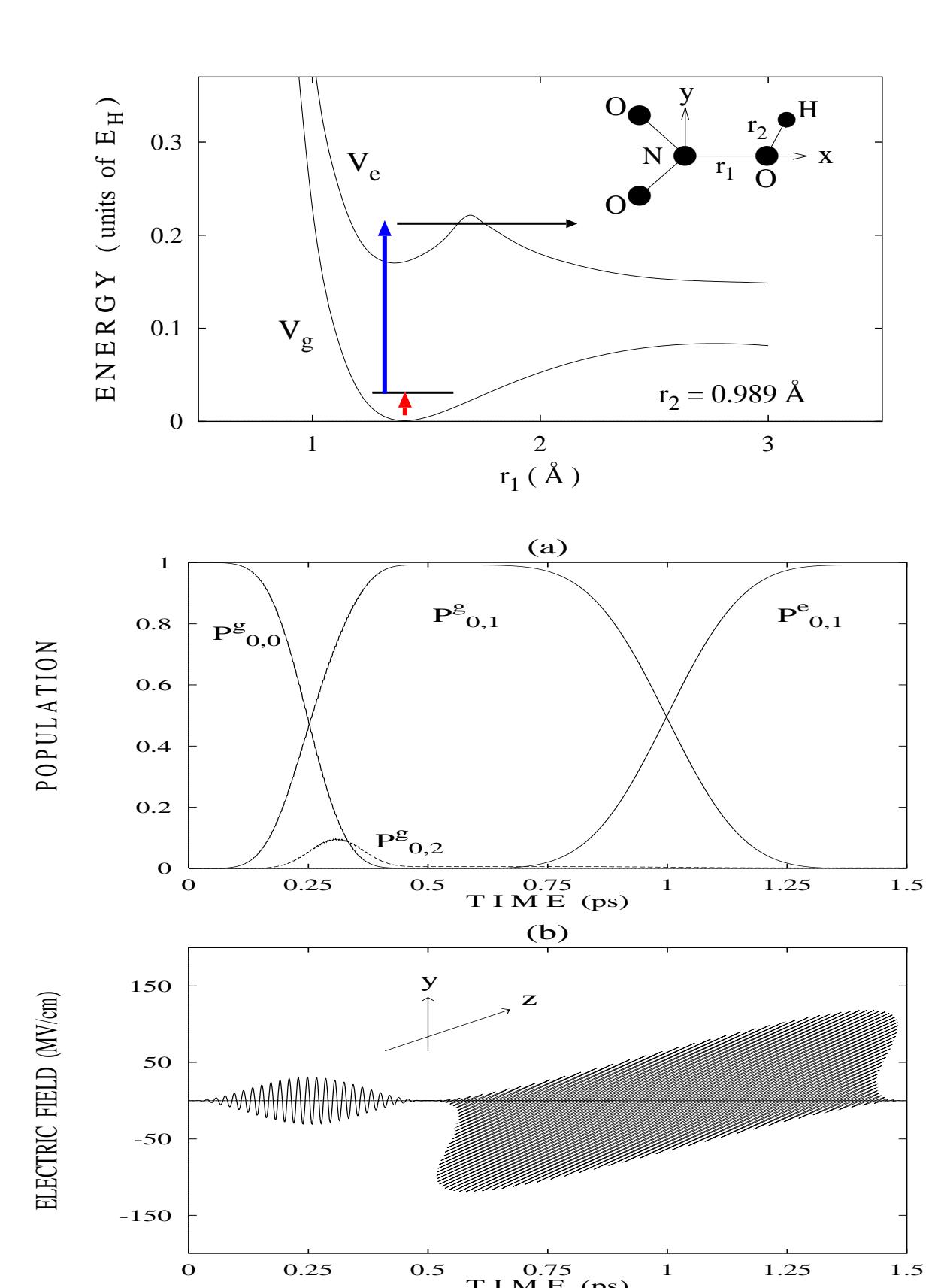


Population vs Time (ps) showing preparation of coherent states.

Laser pulse electric field vs Time (ps).

HONO₂

IR+UV Excitation



Energy levels and intramolecular coordinates \vec{q} .

Population vs Time (ps) showing state preparation.

Electric field vs Time (ps).

Visualising molecular quantum dynamics

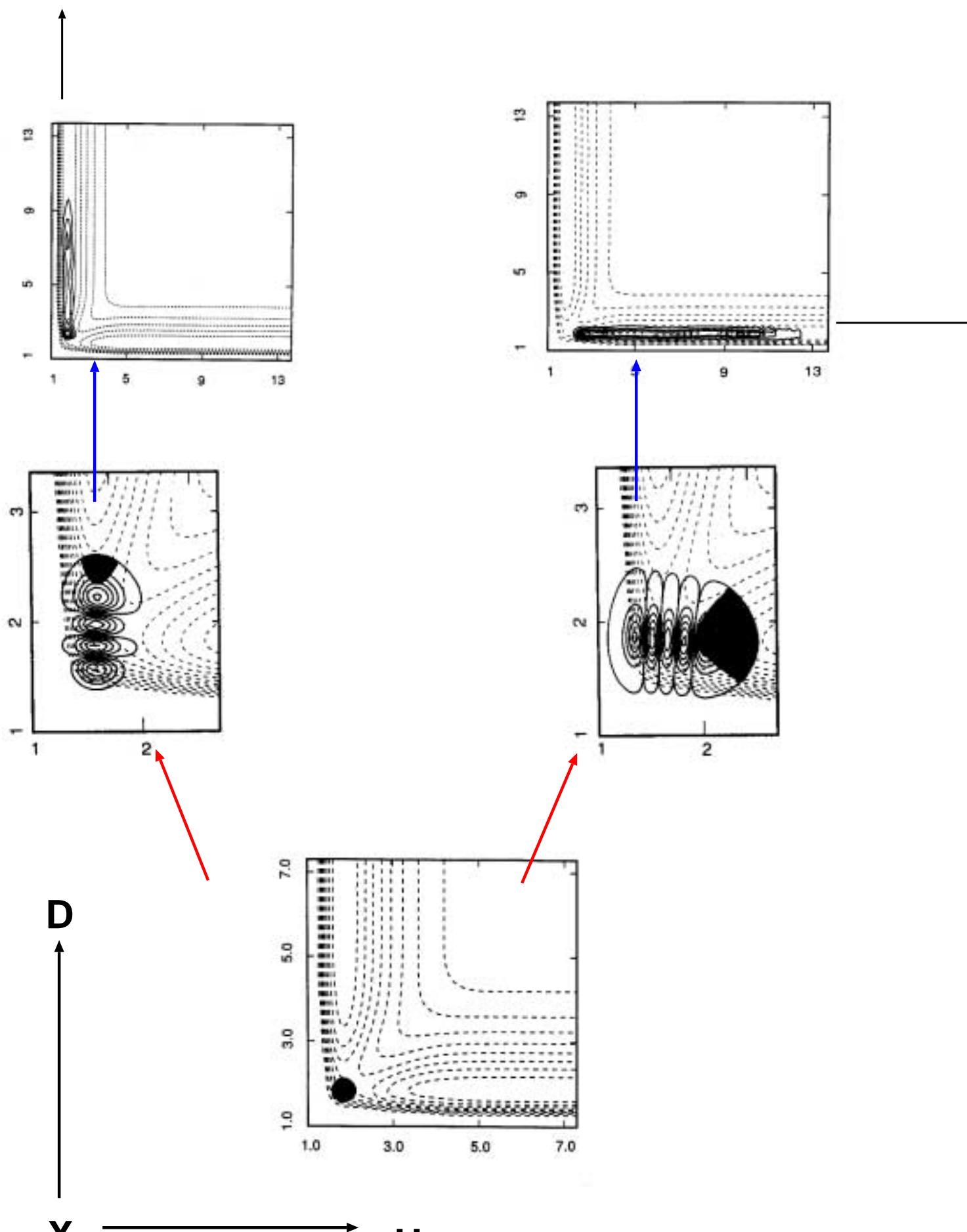
Molecular wavepackets $\Psi(\vec{q}, t) \rightarrow$ molecular quantum dynamics $\rho(x_i, y_i, z_i, t)$

intramolecular coordinates $\vec{q} \rightarrow$ nuclear cartesian coordinates \vec{R}

$\Psi(\vec{q}) \rightarrow \Phi(\vec{R}) = \Psi(\vec{q}[\vec{R}])$

$\rho(\vec{q}) = |\Psi(\vec{q})|^2 \rightarrow \rho_i(x_i, y_i, z_i, t) = \int \int dX_1 dY_1 dZ_1 \dots dX_{i-1} dY_{i-1} dZ_{i-1} dX_{i+1} dY_{i+1} dZ_{i+1} \dots dX_n dY_n dZ_n \rho(\vec{q}[\vec{R}])$

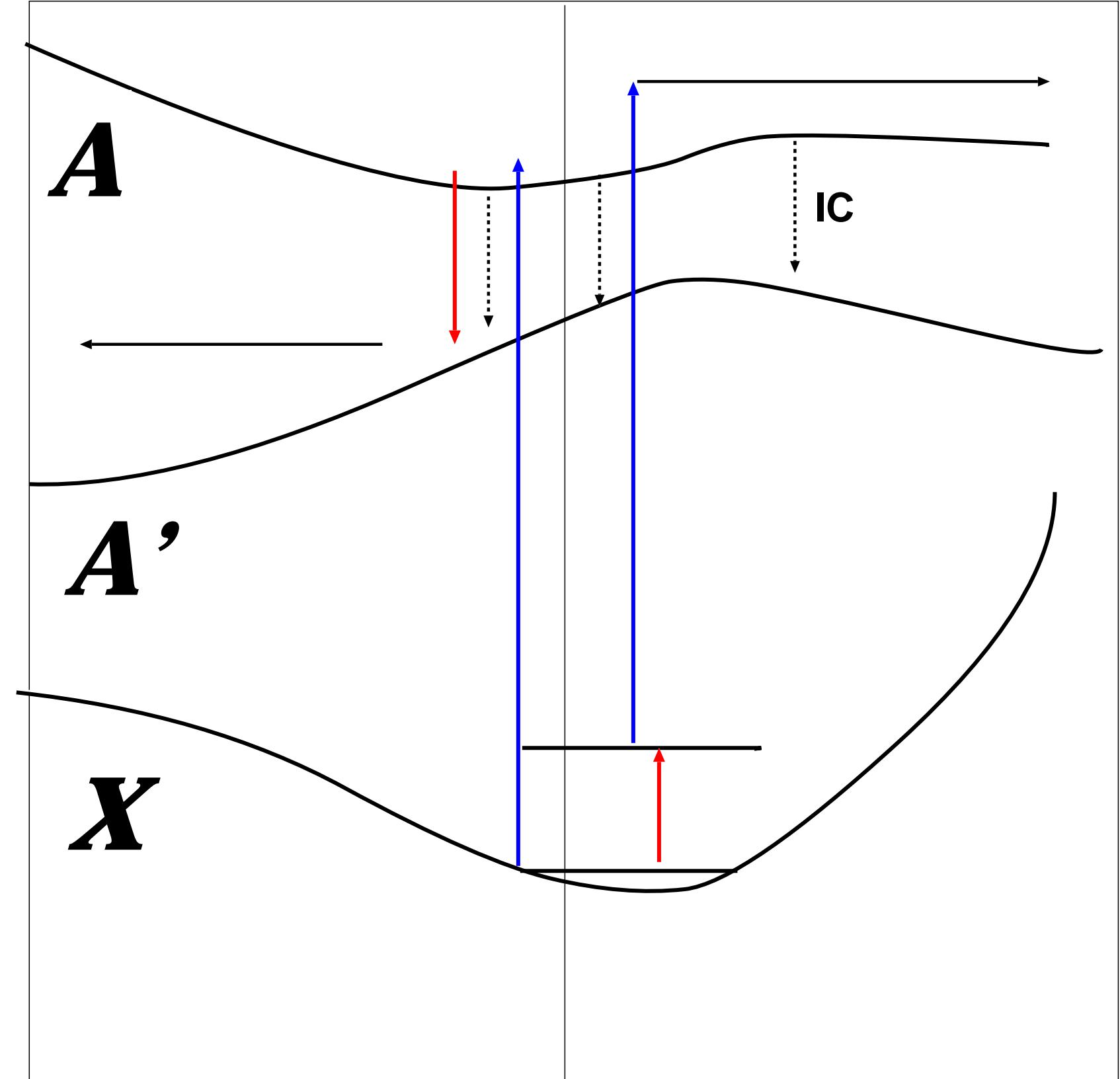
FUTURE



HxD=HOD, HBeD,...

IR-excitation of:
- eigenstates
- zero order states
- coherent states

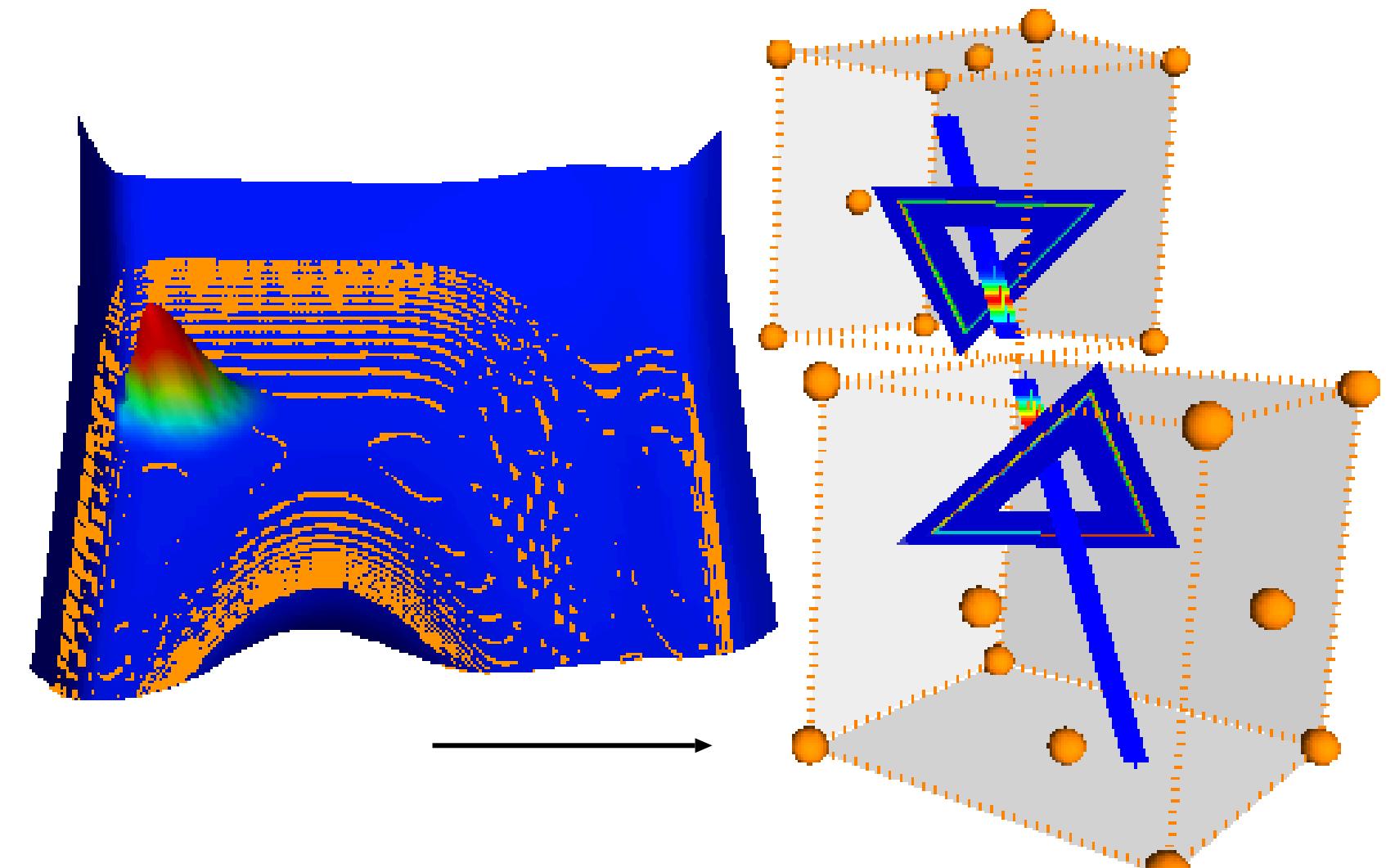
HxD



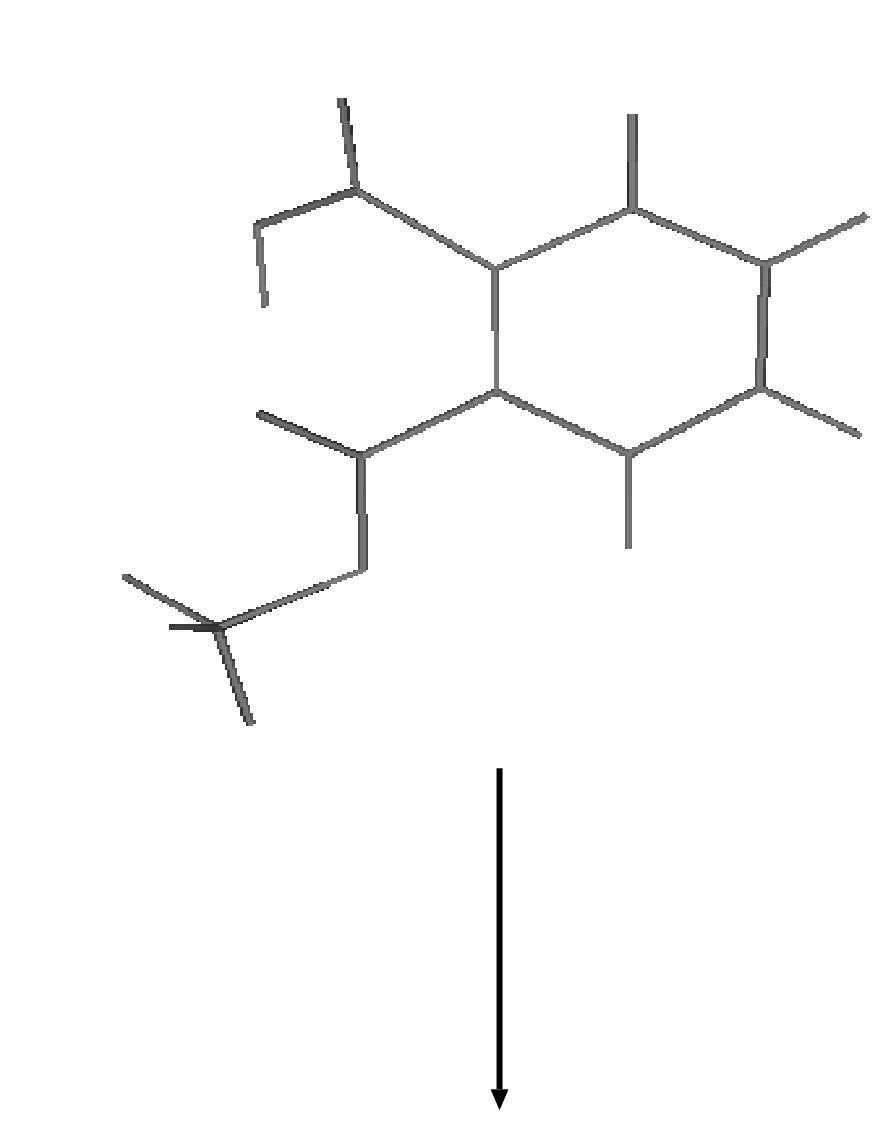
Ba **F** **CH₃**

$\text{Ba} + \text{FCH}_3 \longleftrightarrow \text{Ba...FCH}_3 \longleftrightarrow \text{BaF} + \text{CH}_3$

Example: laser driven cage exit



Example: laser driven hydrogen transfer



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