

Molecular Dynamics for clusters

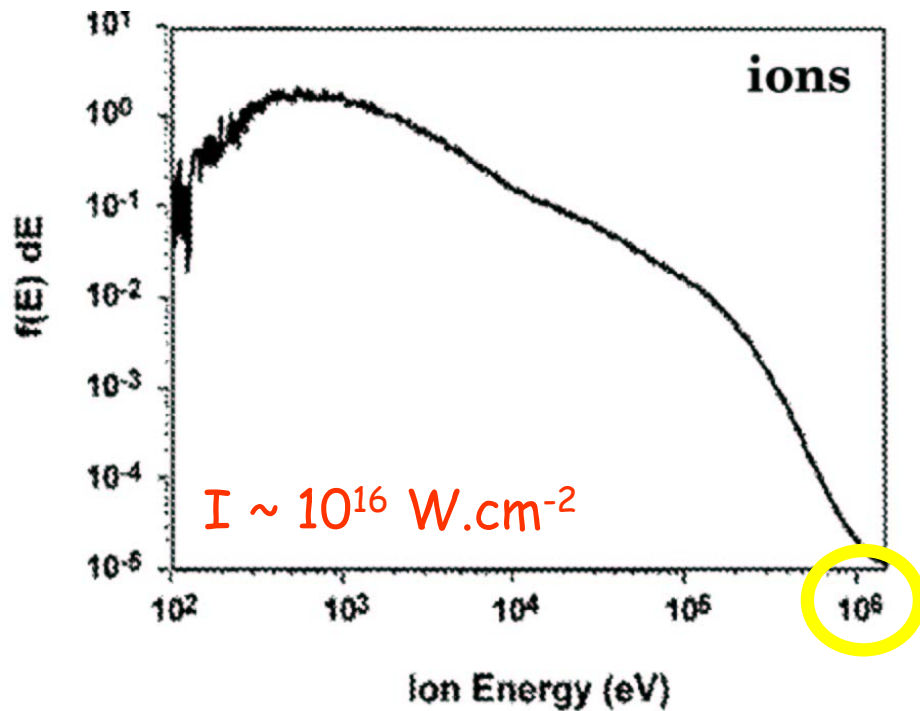
- Classical Molecular Dynamics model for clusters
- Rare gas and metal clusters in high intensity laser fields

- Physical context
- Model and validation
- Clusters in high intensity lasers

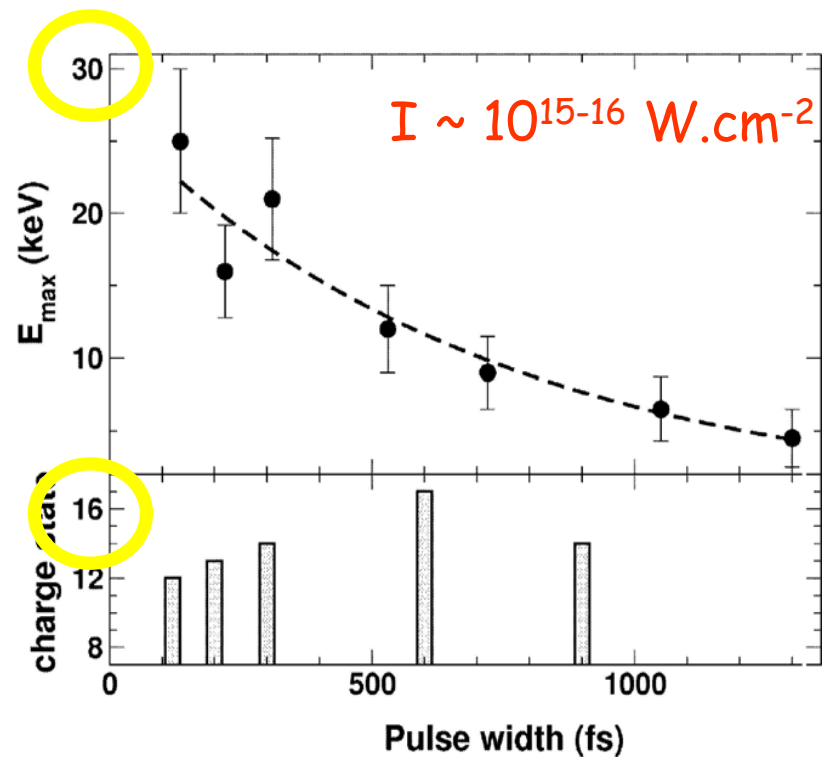
Clusters in high intensity lasers

Xe_{2500}

$Pt_{\sim 50}$



Exp. Ditmire



Exp. Meiwes Brower



Highly charged ions
Huge kinetic energies
X rays, fusion... !

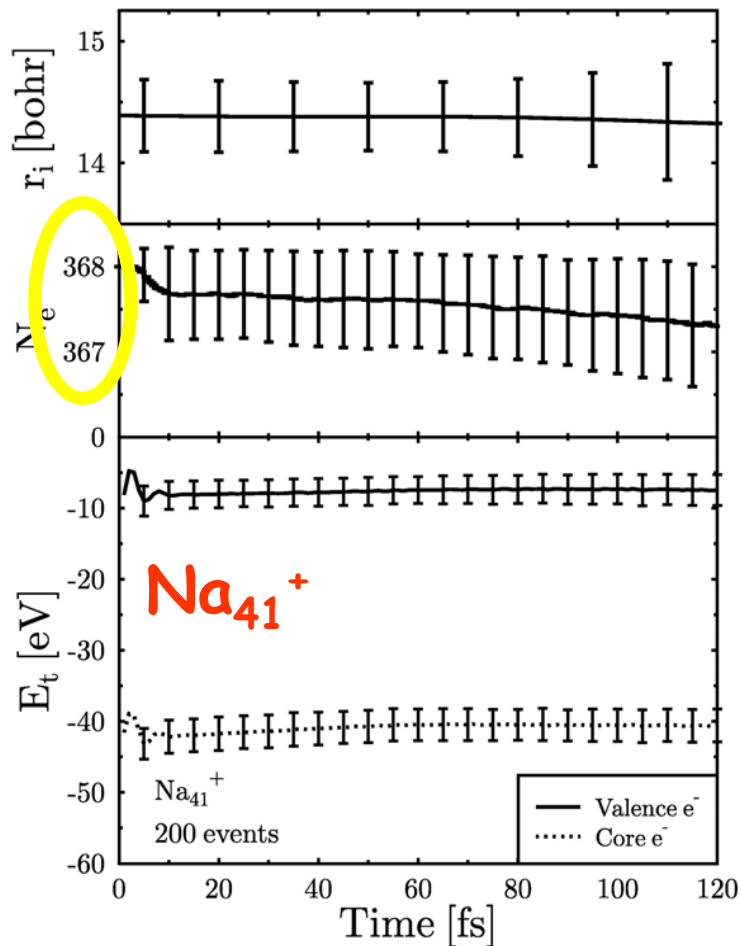
Model : Molecular Dynamics

- Classical treatment of electrons and ions
- Molecular Dynamics (MD) for finite size particles σ_i
 $\{r_i, p_i, \sigma_i\}, i = 1, N$ for both ions and electrons
- Direct Coulomb interaction $\sim e^2 / r_{12}$
- Smooth effective interaction between point particles
 $V_{12} \sim e^2 \operatorname{erf}(r/\sigma_{12}) / r_{12}$ $\sigma_{12}^2 = \sigma_1^2 + \sigma_2^2$
- Classical equations of motion for $\{r_i, p_i\}$ at fixed σ_i 's
 $dr_i/dt = p_i/m$ $dp_i/dt = - \sum_j \nabla_j V_{ij}$
- σ_i 's fitted to electronic sp energies

Ar	(Ne)	$3s^2 3p^6$	8 active electrons	$\sigma_I, \sigma_{3s}, \sigma_{3p}$
Xe	(Kr)	$4d^{10} 5s^2 5p^6$	8 active electrons	$\sigma_I, \sigma_{5s}, \sigma_{5p}$
Na	1s	$2s^2 2p^6 3s$	9 active electrons	$\sigma_I, \sigma_{2s-2p}, \sigma_{3s}$

Ground state stability

Metal cluster

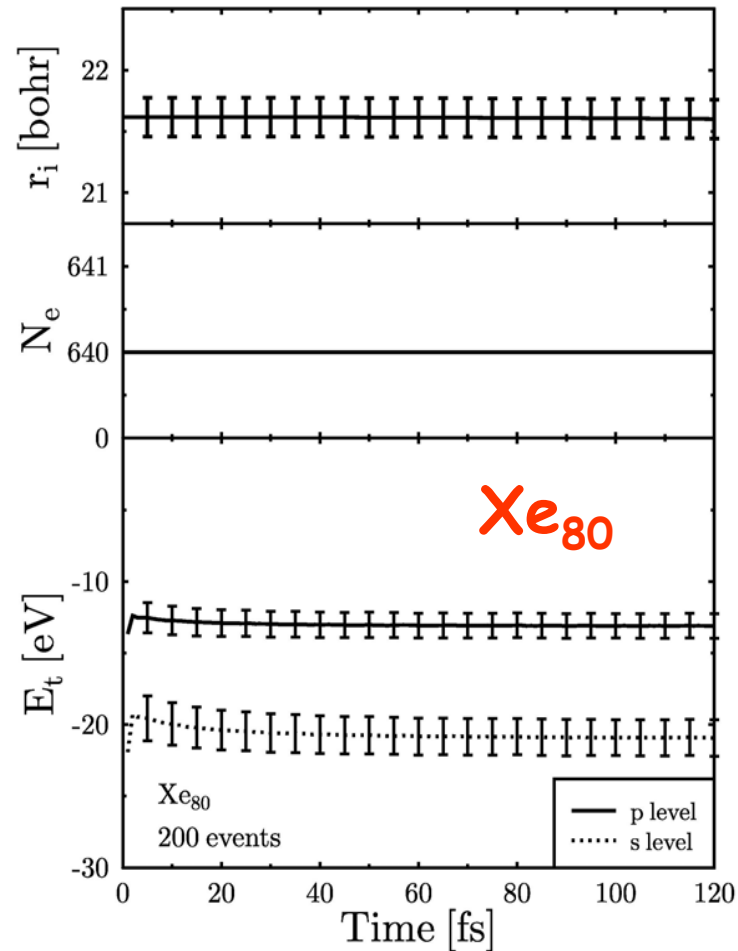


Radius

Ionization

Electron
Energies

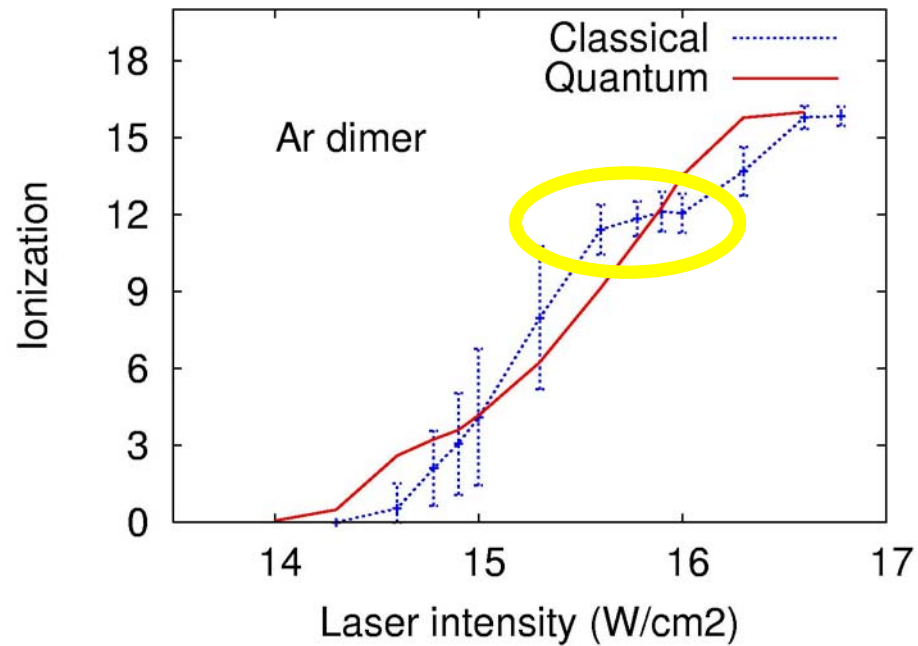
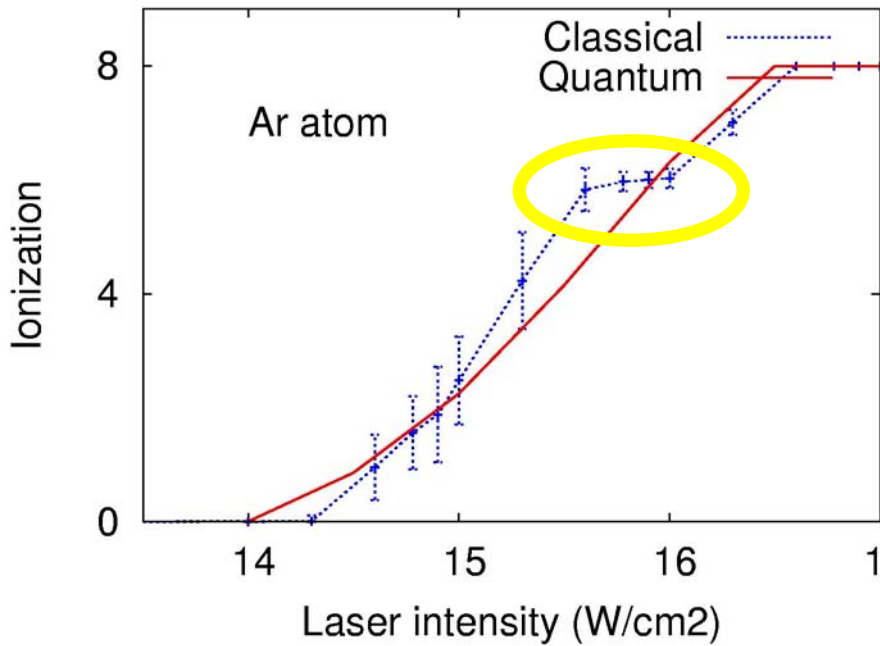
Rare Gas cluster



Good (surprising ?) stability !

Classical vs Quantum dynamics

Emission from irradiated Ar atom or Ar dimer
Comparison of classical (MD) and
quantum (TDLDA, 8 electrons/atom) calculations



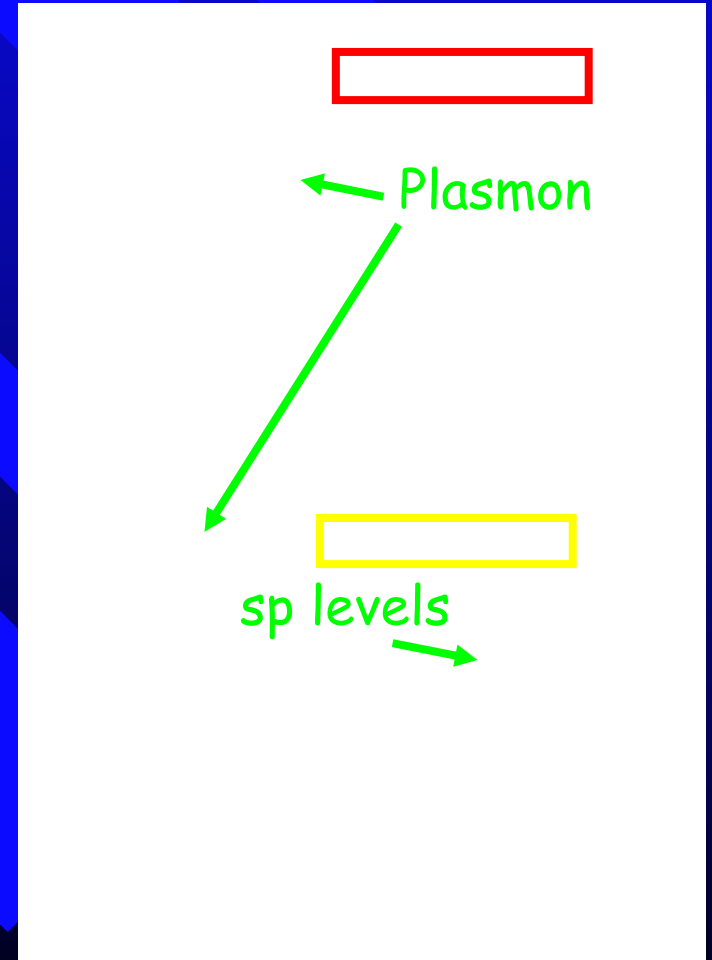
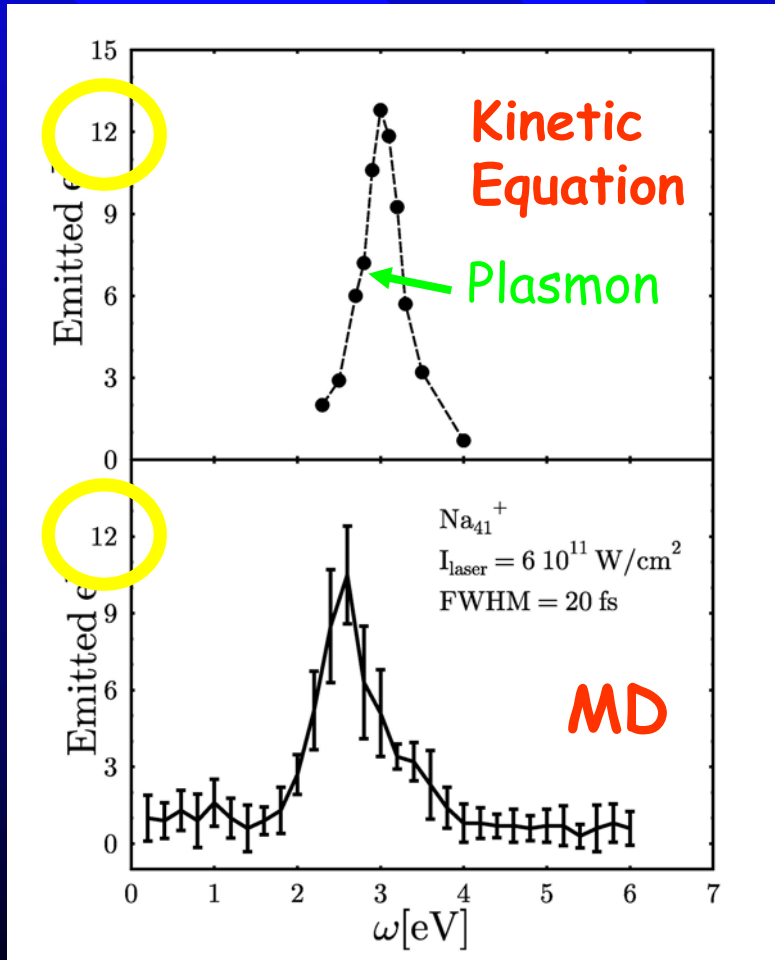
Remarkable agreement !



Linear and semi linear dynamics (metal)

Resonant ionization

Optical response

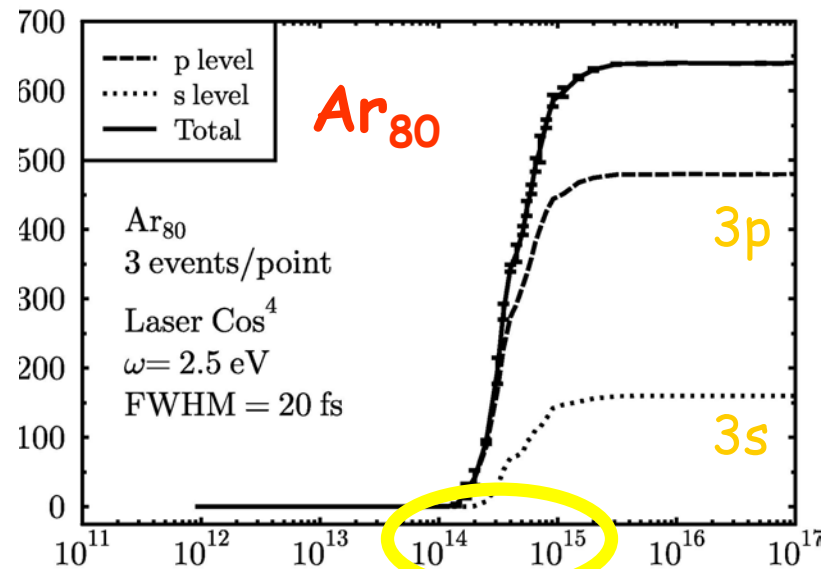
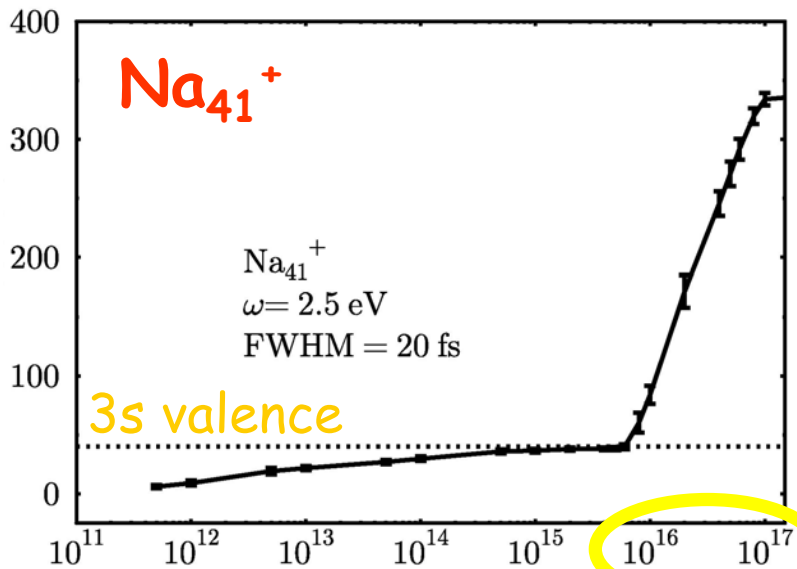


Good agreement : validates MD AND kinetic equation !

Electron emission at high laser intensity

Metal cluster

Rare Gas cluster



Total ionization

Laser intensity $W.cm^{-2}$

Ionization threshold for « deeply » bound states



Coulomb explosion

Question:
Mechanism of explosion ?

Coulomb ? $E_Q \propto Q$

Thermal ? ... $E_Q \propto 1$

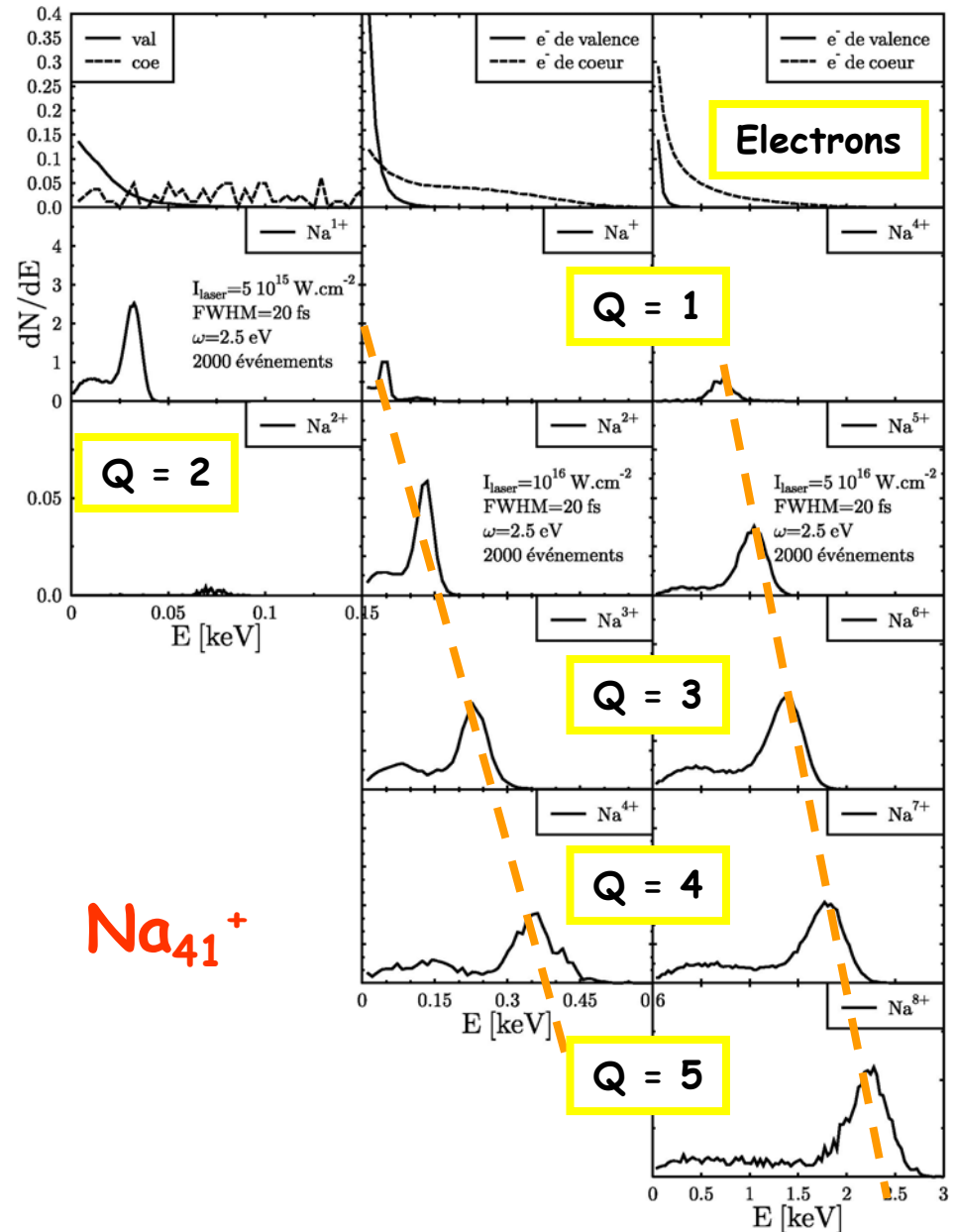


Clear
Coulomb explosion

$I = 10^{15}$

$5 \cdot 10^{15}$

$10^{16} \text{ W.cm}^{-2}$



Na_{41}^{+}

Some conclusions and perspectives

➤ Classical Molecular Dynamics for clusters

Simple stable model

Good properties as compared to semi-classical or quantal results

Applications to clusters irradiated by intense lasers

➤ Many other research directions

- Formal aspects

Ex: quantum vs classical, Pauli principle ...

- Other materials

Ex: Carbon, fullerenes ...

- Mixed quantum/classical treatments

Ex: quantum valence + classical core...

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