2137-38

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Numerical simulation of transport properties in nuclear fuels: from the atomistic scale to the mesoscopic scale

M. Freyss

CEA, Centre de Cadarache
Saint Paul lez Durance
France

Part 2

Numerical simulation techniques for nuclear fuels at the atomistic scale: electronic structure calculations and empirical potentials

Part 2 Outline

***Ab initio* modeling of actinide compounds**
Introduction

- Few words on ab initio methods
- Specificities of actinide compounds
- Results for bulk properties of fuel materials

Empirical potentials for Classical Molecular Dynamics (CMD) modeling of fuels
Introduction

- Various types of potentials
- Results for UO_2

Conclusion

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Atomistic modeling of nuclear fuels

Determine and understand at the atomic scale
- **Physical and chemical properties of fuels**
- **Irradiation effects in fuels**

Decouple basic processes

- Stability of a given type of point defect
- Localization of a given fission product
- Migration mechanism of a chemical element
- Damage created by ballistic collisions
- Fission product segregation
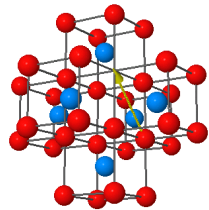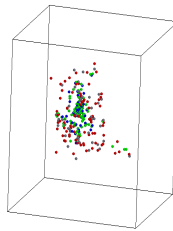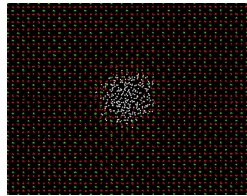
Jmol

Quantify phenomena

- Formation energy of defects
- Incorporation energy of a chemical element
- Structural modification (*swelling*)
- Migration (*migration energy*)
- Concentration of point defects
- Recombining / clustering of defects: nature, size, number
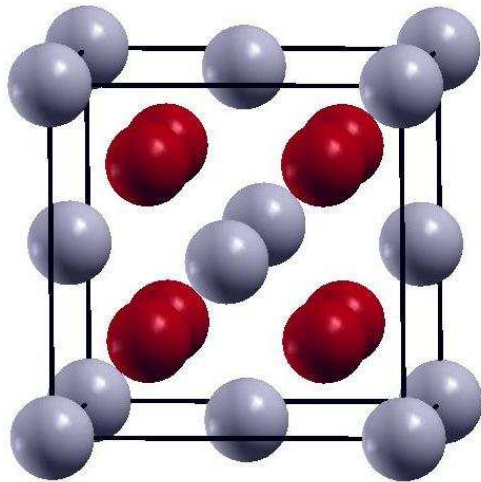
Understanding of the mechanisms involved

Provide basic data for models at a higher scale

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Nuclear materials of interest

actinide dioxides

actinide carbides and nitrides

Fluorite structure
Insulators
Mainly ionic bonding (U^{4+}, O^{2-})

UO_2: a = 5.47 Å
d_{U-U} = 3.87 Å
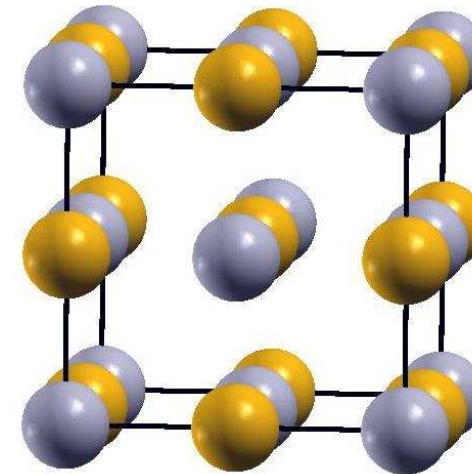
Sodium-chloride structure
Metals
Complex bonding

UC: a = 4.96 Å   **UN**: a = 4.89 Å
d_{U-U} = 3.51 Å d_{U-U} = 3.46 Å

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Atomistic modeling of nuclear fuel

first- principles calculations

empirical potentials
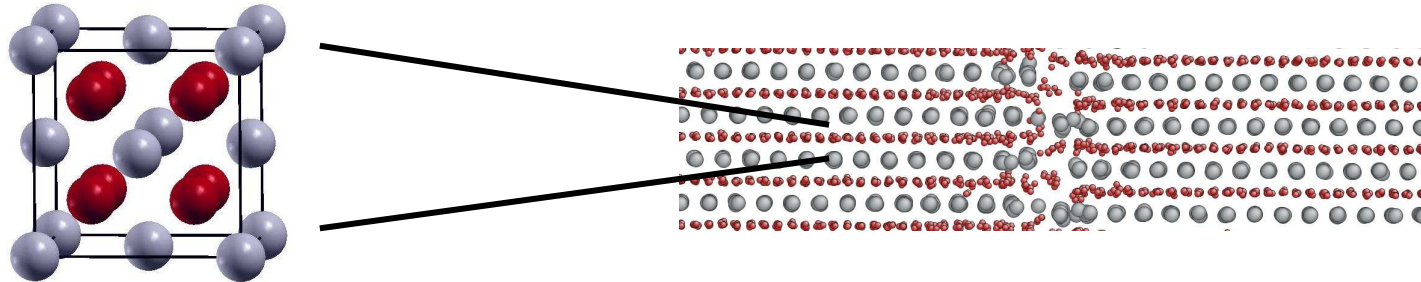
Different scales, different levels of accuracy

Scale: 10 Å (crystal lattice)
~ 100 atoms

Scale: 300 Å (very small grain)
~ 1 000 000 atoms

Forces from electron density
Quantum mechanics

Forces from parametrized
analytical expressions
No electrons

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Ab initio modeling of actinide compounds
Density Functional theory method

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Ab initio modeling: Density Functional Theory method

Description of interaction between nuclei and electrons
Schrödinger equation

$$H \, \Psi(\vec{r}) = E \, \Psi(\vec{r})$$

Impossible to solve for systems with more than 1 electron **!**

Method to solve it: transform it into a single electron problem

Wave function Ψ *for N electrons* → *Wave functions for 1 electron* φ_i

But retain description of the electronic interaction: important in bonding

$$E[n] = T_o[n] + V_H[n] + V_{ext}[n] + V_{xc}[n]$$

kinetic
energy

electrons-
electrons

electrons-
nuclei

**exchange-
correlation**

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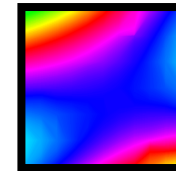# *Ab initio* modeling: Density Functional Theory method

Approximation required for V_{xc}:

⇨ **LDA:** *analytical expression for a uniform electron gas*

⇨ **GGA:** *takes into account the gradient of the electron density*

⇨ **GGA + U:** *addition of parameters to improve the description of strong correlation between 5f electrons*

⇨ **Hybrid functionals:** *GGA + exact exchange*

Choice imposed by the material properties

Iterative self-consistent process

1. Start with guess wave functions φ_i
2. Calculate density
3. Calculate corresponding V_{ext}
4. Solve the approximate equations new φ_i
5. From these calculate a new density
6. Start again

Procedure repeated until convergence is reached
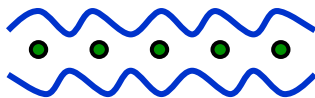
Calculation at 0 K

Ab initio methods expensive in time and computational ressources

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5f electrons in actinide compounds

5f electron spatial <u>localization</u> in the actinide series

UO$_2$: insulator, **localized** *5f* electrons, strong electrostatic interaction underestimated by the DFT

⇨ **GGA + U**

UC, UN: metals, **delocalized** *5f* electrons ⇨ **GGA,** GGA+U?

From Moore *et al.* Rev. Mod. Phys. 81, 235 (2009) and Albers, Nature **410**, 759 (2001).

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Ab initio method for modeling of UO_2 and UC

Projector Augmented Wave method (PAW)
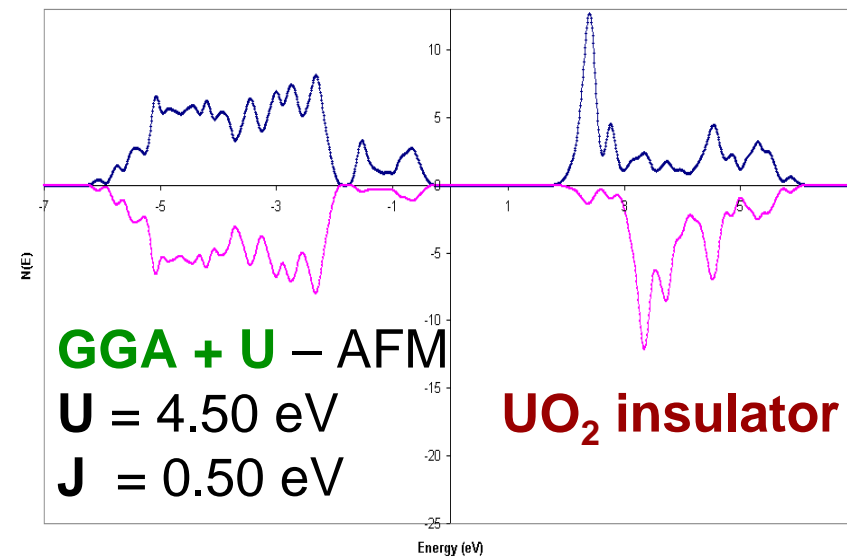
- Based on the Density Functional Theory (**DFT**)
- **Plane-Waves** as basis functions for valence electrons
- **Core electron** density taken into account
- Code **VASP** (http://cms.mpi.univie.ac.at/vasp/)
  Code **ABINIT** (http://abinit.org)
- Scalar relativistic approximation
- Exchange-correlation functional: **GGA** for **UC**
  $\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ **GGA+U** for **UO_2**
- Low **cut-off energy** of the plane-wave basis:
  350 eV for UC, 450 eV for UO_2
- Defects in UC in a **64 atom supercell**
  $\qquad$ in UO_2 in a **96 atom supercell**

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Ab initio modeling of UO$_2$ – GGA / GGA + U

	a (Å)	**B** (GPa)	**C$_{11}$, C$_{12}$, C$_{44}$** (GPa)	**E$_{co}$** (eV)	**m** (μ$_B$/U)
GGA	5.38	184	318, 96, 43	23.3	1.4
GGA+U	5.52	187	382, 130, 54	23.1	2.0
exp.	5.47	207	389, 119, 60	22.0	1.7

*Lattice parameter **a**, bulk modulus **B**, elastic constants **C**,*
*cohesive energy **E$_{co}$**, magnetic moment **m***

GGA – AFM   **UO$_2$ metal**

GGA + U – AFM
U = 4.50 eV
J = 0.50 eV   **UO$_2$ insulator**
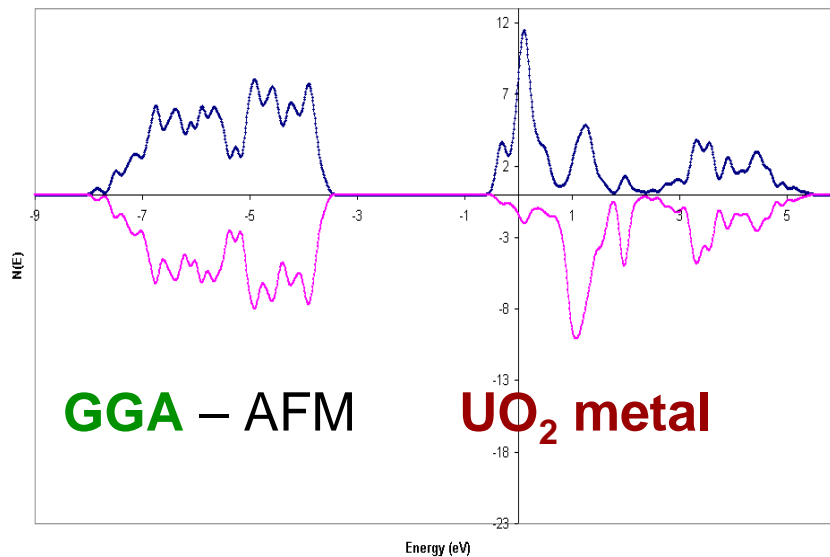
Values of **U and J fixed** to reproduce photoemission data and the 2 eV band gap

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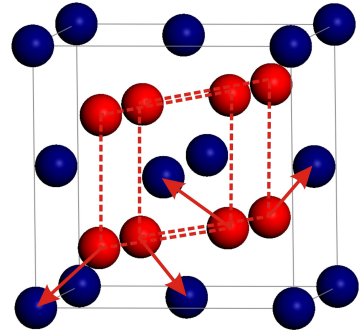CADARACHE

Ab initio modeling of UO$_2$

Many bulk properties of UO$_2$ are difficult to account for by first-principles calculations, or simply make the calculations very long

- *5f* electron **localization** (DFT+U,…)

- **Relativistic** effects (spin-orbit coupling)

- **Non-collinear** magnetic order at low temperatures (T < 30 K)

- **Jahn-Teller** distortion: distortion of the oxygen sub-lattice

- **Large supercells** (~100 atoms) for the study of defects

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Ab initio modeling of UO$_2$

> Below 30 K: stable phase = **Jahn-Teller distorted structure**

Distortion of the oxygen cage

Space group: Pa-3

Non-collinear antiferromagnetic order

> Above 30 K: stable phase = **fluorite structure**
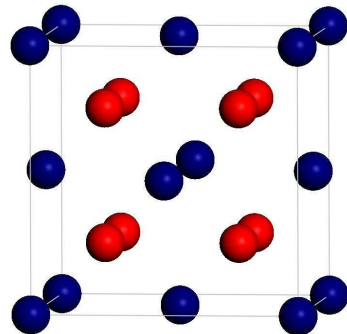
Space group: Fm-3m

Paramagnetism

> Study of point defect behavior **in both phases**

B. Dorado, G. Jomard, M. Freyss, M. Bertolus, submitted (2010)

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DFT+U modeling of UO$_2$

- Uranium atom is surrounded by an oxygen cube and charged 4+
  → electronic configuration: [Rn] 5f^2

- Within DFT+U: orbital localization due to the correction term
  → only two orbitals are filled: **multiple configurations**

State	E (meV/UO$_2$)	Vo (Å^3)	B (GPa)	type (gap eV)	5f occupation
ground state	0	170.29	187	Insulator (2.3)	
1st meta. state	12	170.69	190	Insulator (2.8)	
2nd meta. state	60	170.50	188	Insulator	
3rd meta. state	368	170.64	188	Insulator	
4th meta. state	825	170.18	188	Metallic	

Metastable states

The existence of metastable states can lead to a wrong description of UO$_2$
B. Dorado, B. Amadon, M. Freyss, M. Bertolus, Phys. Rev. B 79, 235125 (2009)

Problem of local minima inherent to approximations which increase the localization
of electrons: **GGA+U**, **Hydrid Functionals** (PBE0, HSE06,…), …

Metastable states also found in **Ce** (Amadon *et al. Phys. Rev. B 77, 155104(2008))*
PuO$_2$, **Pu$_2$O$_3$** *(Jomard et al. Phys. Rev. B 78, 075125 (2008)), …*

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DFT+U modeling of point defects in UO$_2$

Discrepancies for the formation energies of point defects in UO$_2$ from previous studies

Formation energies (eV)	Iwasawa[1]	Gupta[2]	Nerikar[3]	Dorado
Uranium Frenkel pair	13,2	14,2	15,1	13,8

Same PAW method with the GGA+U approximation
[1]. M. Iwasawa *et al.*, Mater. Transac. **47**, 2561 (2006)
[2]. F. Gupta *et al.*, Philos. Mag. **87**, 2561 (2007)
[3]. P. Nerikar *et al.*, J. Nucl. Mater. **384**, 61 (2009)

Wrong description of point defect stability in uranium dioxide if the ground-state electronic structure is not obtained.

One solution is a careful **monitoring of the *5f* occupation matrices** in order to make sure that the ground-state is reached.
B. Dorado, G. Jomard, M. Freyss, M. Bertolus, submitted (2010)

To be checked for other nuclear fuel materials too, like **(U,Pu)C**, **(U,Pu)N**

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Ab initio modeling of UO$_2$, UC, UN, PuC

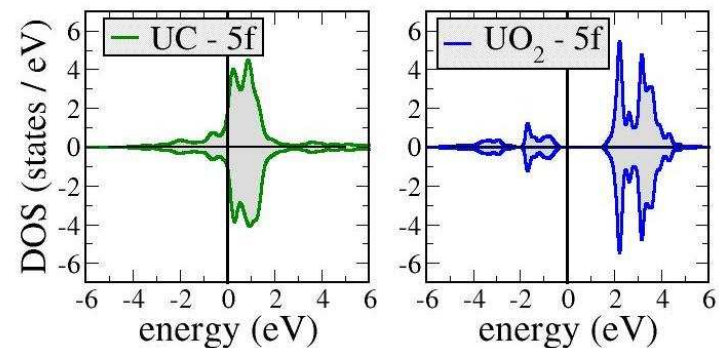## Comparison calculation / experimental data

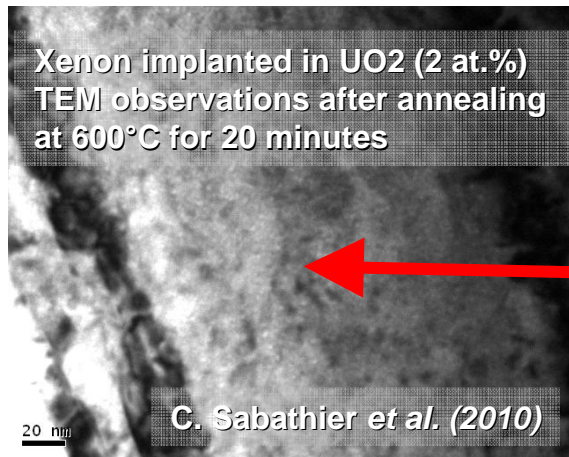Lattice parameter **a**   Bulk modulus **B**   Elastic const. **C**

GGA-PBE	**a** (Å)		**B** (GPa)		**C$_{11}$, C$_{12}$, C$_{44}$** (GPa)	
	calc	**exp**	**calc**	**exp**	**calc**	**exp**
UC GGA	4.93	4.96	185	167	286,135,20	330,86,64
UC GGA+U *(3 eV)	4.98		192		315,136,72	
UN GGA	4.87	4.89	216	194	/	412,84,76
UO$_2$ GGA+U	5.52	5.47	187	207	382,130,54	389,119,60
PuC GGA	4.97	4.97	126	/	/	/

* H. Shi, Phys. Lett. A 373, 3577 (2009)

- **UC metallic:** *5f* states at the Fermi energy, like UN
- Lack of experimental data for **PuC**

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Evaluation of the DFT accuracy for rare gases

Xenon implanted in UO2 (2 at.%)
TEM observations after annealing
at 600°C for 20 minutes

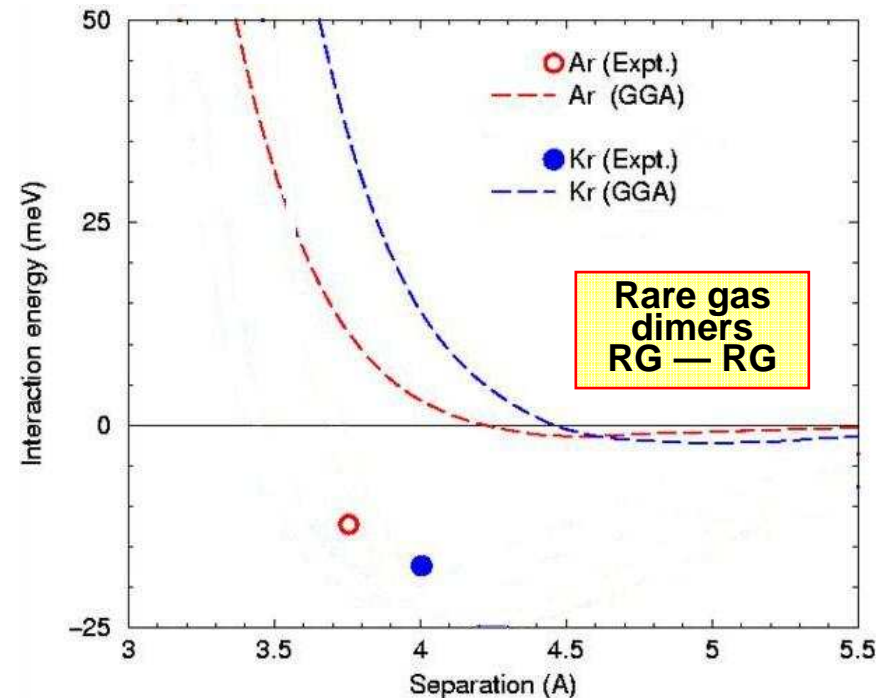C. Sabathier *et al.* (2010)

20 nm

Rare gases (Xe, Kr): most abundant fission products

Xenon bubble formation
Ø 2 nm ~ 100 xenon atoms

Ab initio investigation of solids: DFT

- Current DFT functionals (LDA/GGA): no description of **dispersive Van der Waals bonds**. Fail to describe rare-gas solids, rare-gas clusters…

- Evaluation of DFT accuracy for **bonds formed between rare gases and open-shell atoms** using standard functionals

Improvement: Non-local correlation functionals (vdW-DF, VV09…) not yet available in solid codes (VASP, ABINIT…)

- Ar (Expt.)
- Ar (GGA)
- Kr (Expt.)
- Kr (GGA)

Rare gas dimers RG — RG

From Langreth *et al.* J. Phys.: Condens. Matter **21,** 084203 (2009)

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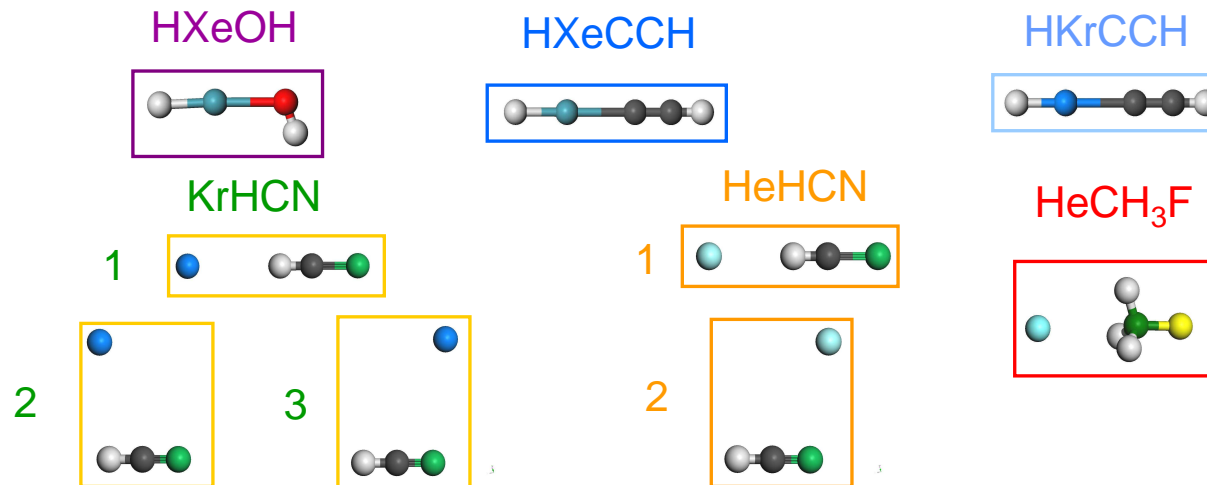
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Evaluation of the DFT accuracy for rare gases

DFT study of small molecules containing rare gas
by M. Bertolus (CEA-Cadarache)

- Experimental data available
- Very precise post-HF calculations feasible (CCSD(T), VTZ+P basis set)
- Molecular codes: Gaussian, Molprol, DMol
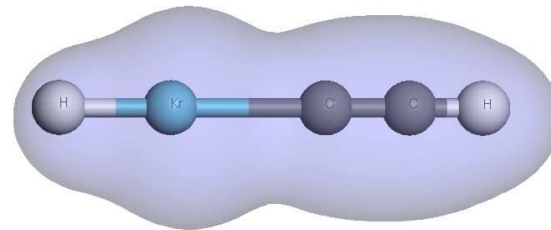- Functionals: LDA, GGA, hybrids

HXeOH

HXeCCH

HKrCCH

KrHCN

1

2

3

HeHCN

1

2

HeCH$_3$F

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Evaluation of the DFT accuracy for rare gases

XeOH, HXeCCH and HKrCCH

- Short RG – X bonds: comparable to distances in solids
- Strong interactions: sharing of electronic density
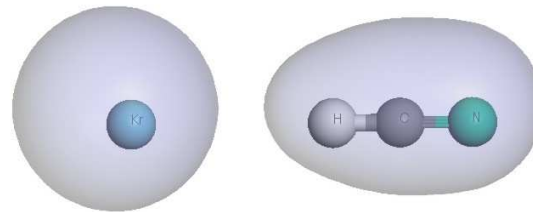- DFT: good geometries, reasonable energies and vibration frequencies

HKrCCH

KrHCN, HeHCN and HeCH$_3$F

- Weak interactions (~ 1-10 meV) and long bonds: dispersion
- Mediocre results for KrHCN, poor for He compounds
- No LDA, GGA or hybrid functional give consistent results

KrHCN

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Empirical Potentials and Classical Molecular Dynamics Simulations of Nuclear Fuels

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Empirical potentials

Principle

- Interatomic interactions described by analytical potential giving the energy as a function of the separation distance
- Parametrized on experimental and *ab initio* data
- Potential form different for each system type
- Parameters different for each system

Advantages / Disadvantages

- Quick ⇨ Investigation of large systems / long times
- Existing data necessary for parametrization
- Non transferable: potentials only valid in situations close to those used for the parametrization
- No description of the electronic structure

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Molecular Dynamics Simulation

Principle

⇨ Computer simulation using Newtonian mechanics

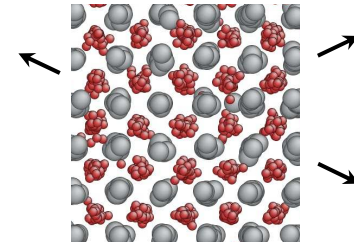$F_A = \sum_i F_{i \rightarrow A}$ et $F_A = m_A \ddot{x}_A$

⇨ Simulates evolution of systems in time

⇨ Enables to find the properties of complex systems numerically

⇨ Based on statistical mechanics

⇨ Calculation in a statistical ensemble (example: N, V, T constant)

⇨ Calculations at finite temperature

Different types depending on the description of atomic interaction

⇨ Empirical potentials: classical molecular dynamics

⇨ *Ab initio* description: *Ab initio* molecular dynamics

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Types of empirical potentials

The analytical form of the potential is defined by the **nature of the bonding**:

- **Covalent**: **Morse** $V(r) = D\left\{\left[1 - \exp\left(\beta\left(r - r_{ij}\right)\right)\right]^2 - 1\right\}$

  Tersoff

- **Metallic**: Modified Embedded Atom Method (**MEAM**) potential

- **Dispersive**: **Lennard-Jones** $V(r) = \dfrac{A}{r^{12}} - \dfrac{B}{r^6}$

- **Ionic**: **Born-Mayer**   **Buckingham**

  $V(r) = A \exp\left(-\dfrac{r}{B}\right)$ $V(r) = A \exp\left(-\dfrac{r}{B}\right) - \dfrac{C}{r^6}$

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Types of empirical potentials

Pair potentials

$$U = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} V(r_{ij})$$

relative distance between 2 ions

<u>Two categories</u>:

- **Rigid ions model** : massive point charges.

Different parametrizations for the Buckingham UO_2 potentials:
Lewis-Catlow, Morelon (**CEA**), Arima, Basak, Yakub
(Comparison in Govers *et al.* J. Nucl. Mater. 366, 161 (2007) and
Devanathan *et al.*, J. Chem. Phys. 130, 174502 (2009))

- **Core-shell model** (polarizability): ions described by a massless charged shell bound to a massive core by a spring. Interatomic potentials act on the shells (Coulomb interaction acts on both shells and cores).

Better fit of the core-shell model to experimental bulk properties of UO_2 (phonon spectrum for instance) than the rigid ion model, but higher computational cost. Not used for collision cascades.
Comparison rigid-ion / core-shell model on bulk properties of UO_2 in Govers *et al.* J. Nucl. Mater. 366, 161 (2007)

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Types of empirical potentials

Many body potentials

$$U = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} V(r_{ij}) + \sum_{i}^{N} U(\rho_i)$$

$$\text{with} \quad \rho_i = \sum_{j=1, j \neq i}^{N} f(r_{ij})$$

Various types of potentials exist depending on the analytical form of *f* and *U*

Examples:

Tersoff Tersoff, Phys. Rev. B 39, 5566 (1989)

Ge nanoparticles, Pizzagalli *et al.* Phys. Rev. B 63, 165324 (2001)

EDIP (environment-dependent interatomic potentials)

Bazant *et al.*, Phys. Rev. B 56, 8542 (1997)

SiC with defects, Lucas *et al.,* J. Phys.: Condens. Matter 22, 035802 (2010)

MEAM (modified embedded atom method) Baskes, Phys. Rev. B 46, 2727 (1992)

δ-Pu lattice vibrations, Baskes *et al.,* Phys. Rev. B 72, 014129 (2005)

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Empirical rigid-ion pair potentials for UO_2

$$V_c(r) = \frac{1}{4\pi\varepsilon_0}\frac{e^2 Z_i Z_j}{r}$$ coulombic term

Buckingham $$V(r) = A\exp\left(-\frac{r}{B}\right) - \frac{C}{r^6}$$

short-range repulsion   long-range dispersion

Various possible parametrizations (**A, B, C, Z**) for UO_2

U-U interactions purely coulombic ($A_{UU}=C_{UU}=0$, CEA potential), or not.

Dispersion only for O-O interactions ($C_{UO}=C_{UU}=0$).

Additional repulsive term (Ziegler-Biersack-Littmark ZBL) for very short distances, required for collision cascade simulations.
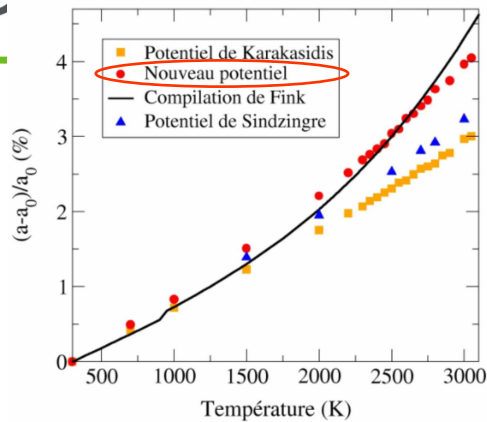
Z non-integer (CEA potential: $U^{+3.227}$, $O^{-1.614}$). Fixed charges for each ion.

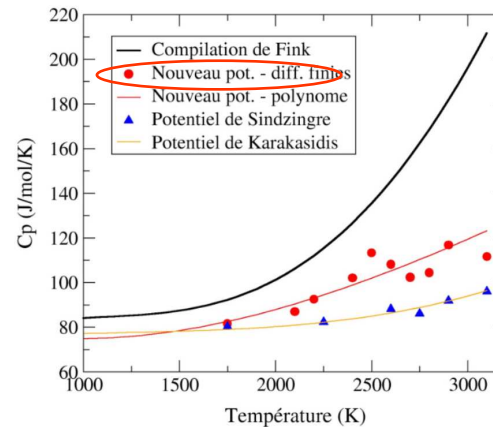Morse-type covalent interaction term added for U-O interactions, or not (CEA potential)
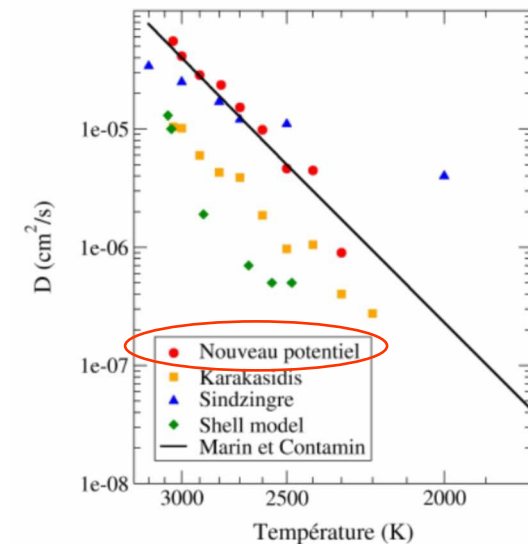
Empirical potentials for UO$_2$

Thermal expansion

Heat capacity

Oxygen diffusion

Energy [eV]	Experimental	Ab-initio 1	Ab-initio 2	Rigid ions Karakasidis	Rigid ions Morelon
Formation Frenkel O	3.5±0.5	3.8	3.7	4.37	3.17
Migration vac. O	0.5		1.2	0.14	0.33
Migration int. O (direct)	0.8 - 1.0		3.6	0.43	1.37
Migration int. O (indirect)			1.1	0.07	0.65
Formation Frenkel U	9.5	10.7	9.0	16.53	12.6
Migration vac. U	2.5		4.4	5.1	4.46
Migration int. U	2.0		5.8	5.3	5.0
Formation Schottky	6.5±0.5		5.2	5.08	6.68

For simulation of displacement cascades initiated by a recoil nucleus, the potential are fitted to reproduce not only physical and thermoelastic properties but also the energies of formation and migration of point defects.

1 J.P. Crocombette *et al*. Phys. Rev. B 64, 104107 (2001)
2 M. Freyss *et al*. J. Nucl. Matter. 347, 44 (2005)

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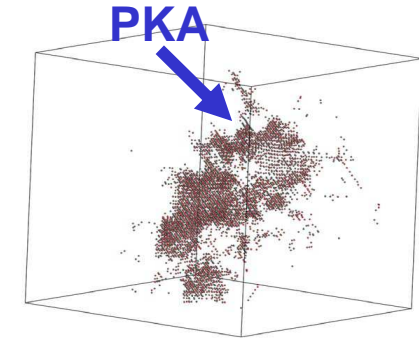# Irradiation damage: comparison of empirical potentials

Average number of defects in UO$_2$ after a collision cascade with a uranium primary knock-on atom (PKA) of 1 keV

Number of Frenkel pairs created
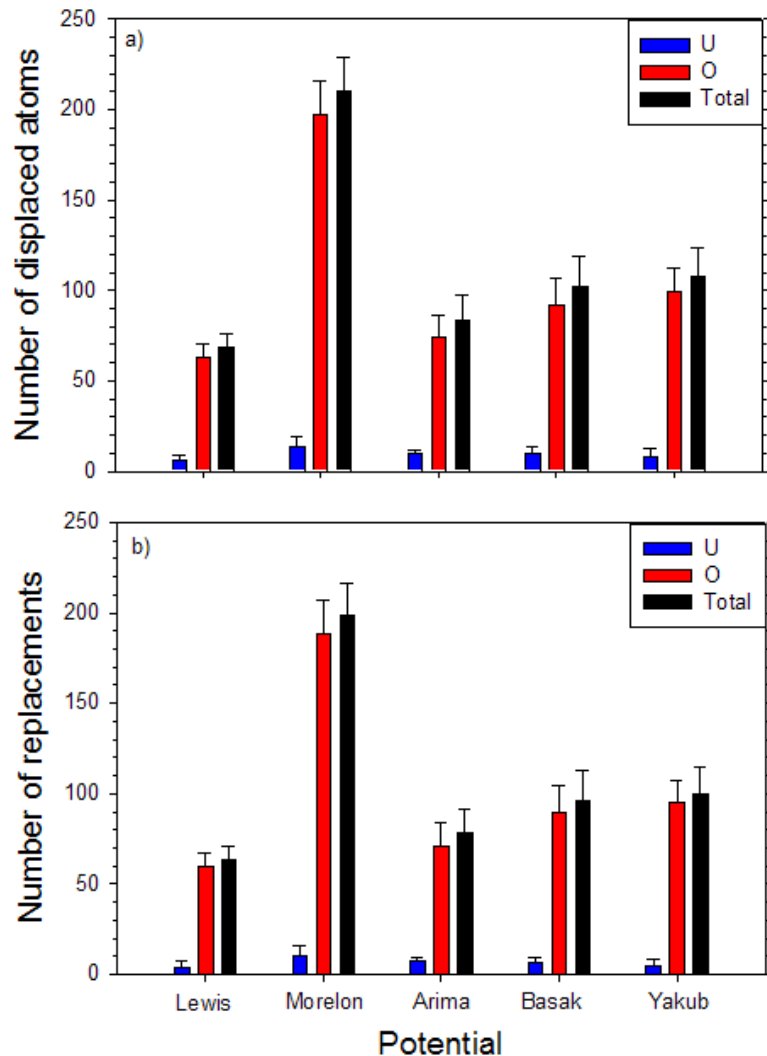(1 interstitial + 1 vacancy of the same chemical element)
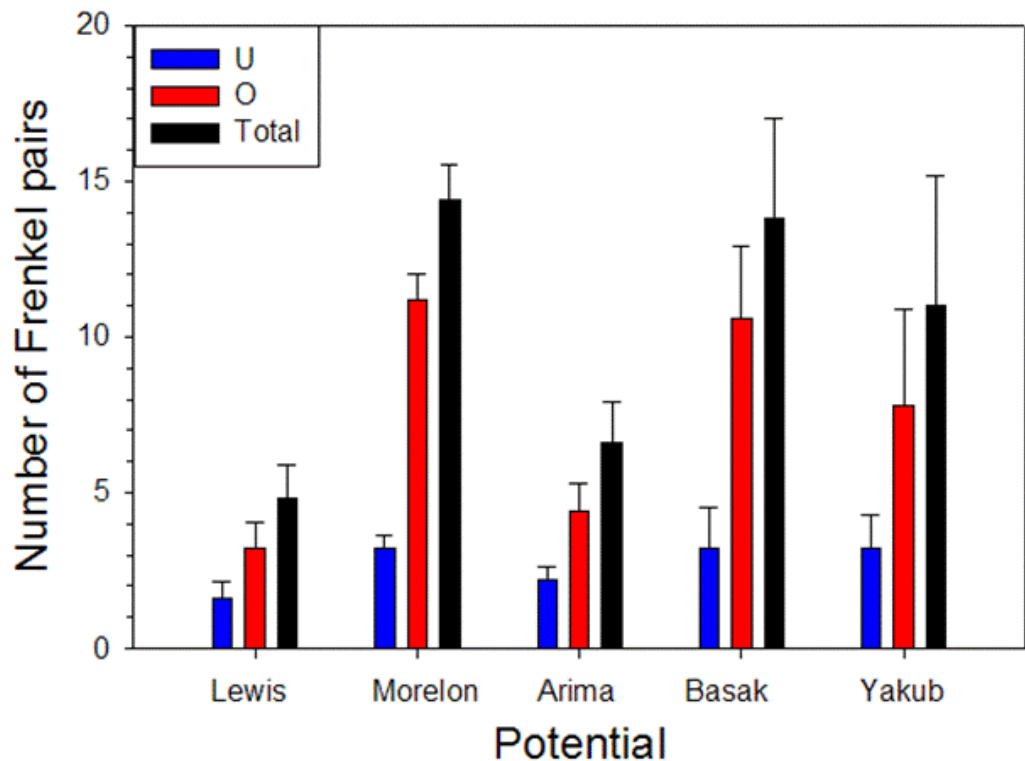
Number of defects O/U ~2 for all potentials. Neutral defects

Same behavior for U with all pair potentials, but some differences for the O sub-lattice

Oxygen mobility is the main difference between the potentials

From Devanathan *et al.* J. Chem. Phys. 130, 174502 (2009)

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Irradiation damage: comparison of empirical potentials

Number of defects created after a collision cascade with a uranium PKA of 1 keV (number of atoms displaced at least 2 Å from their lattice site)

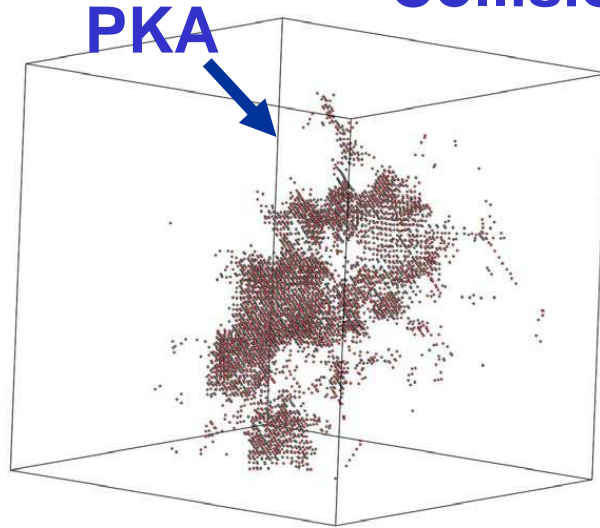Same trends for all potentials: more O atoms displaced than U atoms.

Differences in the number of defects created but the number of replacements is 90-95% of the displaced atoms (recombination).

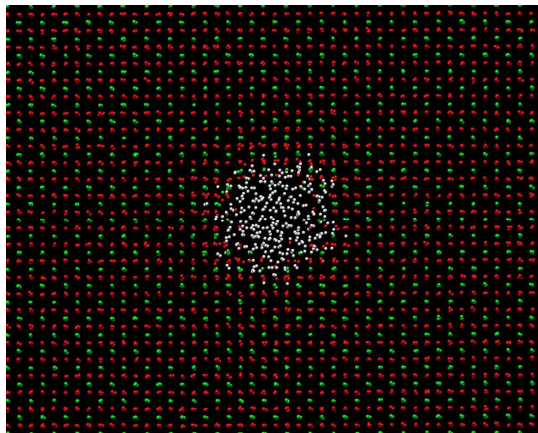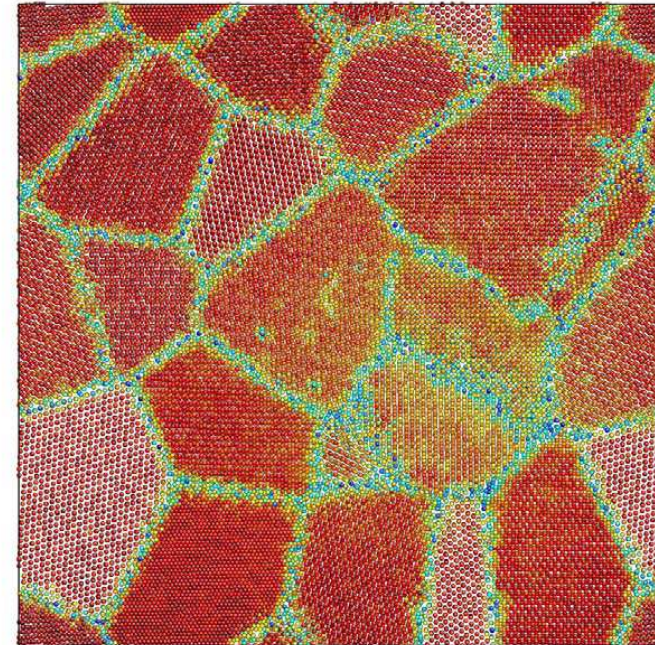From Devanathan *et al.* J. Chem. Phys. 130, 174502 (2009)

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Studies of UO$_2$ with empirical potentials

Collision cascades

PKA

Defects at grain boundaries

Gas bubble nucleation

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Part 2 Conclusion

Application of atomistic calculations to nuclear fuels

- Ab initio calculations and CMD simulations are powerful tools
  - to identify atomic scale mechanisms
  - to generate quantitative data
- Studies of phenomena difficult to access experimentally
- Support experiments and microscopic modeling techniques

Challenges for the future

- Better *ab initio* approximation of strong correlation in UO_2
- Better *ab initio* description of Van der Waals interactions to model rare gases in the material
- Development of empirical potentials for rare gases & fission products
- Improve the potentials for UO_2 (better fit for non equilibrium conditions, charge fluctuations, N-body terms, …)
- Dynamic simulations for larger time scales (temperature accelerated dynamics TAD)

- Better integration of *atomistic* calculations in the **multiscale** modeling of nuclear fuels

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Acknowledgements

CEA Cadarache / Fuel Study Department

<u>From the lab</u>: C. Valot (head), M. Bertolus, B. Dorado, G. Martin, P. Garcia, P. Martin, G. Carlot, C. Sabathier, J. Durinck, C. Davoisne, M. Fraczkiewicz, H. Palancher, C. Martial, J.C. Dumas, J.P. Piron,

<u>From the department</u> : B. Pasquet, B. Michel, A. Bouloré, L. Noirot, P. Obry, Y. Guerin

CEA Saclay H. Khodja, C. Rapsaet, L. Van Brutzel, A. Chartier, JP. Crocombette, C. Gueneau
CEA Saclay – Ecole Centrale – CNRS : G. Baldinozzi, D. Siméone, C. Petot
CEA DAM F. Jollet, B. Amadon, G. Jomard, M. Torrent, F. Bottin
IRSN: R. Ducher

Imperial College (UK): R. Grimes, D. Parfitt
CNRS (F): MF. Barthe, T. Sauvage, P. Desgardin, E. Gilabert, F. Garrido
ITU (D): R. Konings, J. Somers, E. Kotomin, D. Gryaznov, P. van Uffelen, T. Wiss
SCK-CEN (B): K. Govers
NRG (NL): S. De Groot
ESRF FAME BL (F): O. Proux, J.-L. Hazemann, V. Nassif
TUM (D): N. Wieschalla, W. Petry, R. Jungwirth
AREVA-CERCA (F): C. Jarousse

ACTINET network of excellence

F-BRIDGE European project

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