energies on these surfaces, analyzing as well the position of the vacancy formation on the surface. We find that the work to create an oxygen vacancy at such surfaces is not directly related with the relative ordering of the surface stabilities. We also give an explanation for the cluster of oxygen vacancies formation on the (110) surface, including the vacancy monomer, dimer, and trimer, showing that the linear vacancy formation is the most stable vacancy formation. Furthermore, we have studied the adsorption of H2O and H2 on different sites of the (110) surface, computing the dissociation energy of these molecules. The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement No. 269903.

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16:00 **Phonon spectrum, thermal expansion and heat capacity of UO2 from first-principles** 4 6

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Resume : With the aim to study thermal properties of the nuclear fuel material uranium dioxide, we have performed ab-initio calculations of its phonon dispersion spectrum, thermal expansion, and heat capacity. The so-called direct method, based on the quasiharmonic approximation, is used to calculate the phonon frequencies within a density functional framework for the electronic structure. The phonon dispersions calculated at the theoretical equilibrium volume agree well with experimental dispersions. The computed phonon density of states compare reasonably well with measured data, as do also the calculated frequencies of the Raman and infrared active modes including the LO/TO splitting. To study the pressure dependence of the phonon frequencies we calculate phonon dispersions for several lattice constants. Our computed phonon spectra demonstrate the opening of a gap between the optical and acoustic modes induced by pressure. Taking into account the phonon contribution to the total free energy of UO2, its thermal expansion coefficient and heat capacity have been computed, and are found to be in good agreement with available experimental data for temperatures up to about 500K. Our results exemplify the feasibility of performing first-principles modeling of the thermal properties of this important nuclear fuel material.

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16:00 **EURATOM FP7 Collaborative Project FIRST-Nuclides** 4 7

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Resume : With respect to the fast/instant release of radionuclides from spent nuclear fuel under deep underground repository conditions, a series of questions are still open. These questions concern key input data to safety analysis, such as "instant release fraction (IRF)" values of various radionuclides. In the present communication we report on the EURATOM FP7 Collaborative Project "Fast/Instant Release of Safety Relevant Radionuclides from Spent Nuclear Fuel (CP FIRST-Nuclides)", which started in January 2012 and has a duration of three years. The project is established with the overall objective to provide for improved understanding of the fast / instantly released radionuclides from disposed high burn-up UO2 spent nuclear fuel. The dependence of the IRF on critical characteristics of the spent nuclear fuel (e.g. manufacturing process, burn-up history and fuel temperature history, ramping processes and storage time) are studied in detail. The project provides for experiments combined with modeling studies on integration of the different results as well as for up-scaling from experimental conditions to entire LWR fuel rods. Experimental facilities with specialized equipment for work with highly radioactive materials collaborate for improving the knowledge relevant for the period after losing of the disposed canister integrity. The project is implemented by a consortium with ten beneficiaries (AEKI/MTA, AMPHOS21, CNRS, CTM, FZ Juelich, JRC-ITU, KIT, PSI, SCK/CEN and STUDSVIK).

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16:00 **Characterisation of Depleted Uranium Particles from a Test-Firing Range Using Secondary Ion Mass Spectrometry** 4 8