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DFT calculations of Ti-based molecules clustering with Ar for laser-based enrichment of stable isotopes

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The selective production of radioisotopes with low-energy particle accelerators based on fusion-evaporation reactions, or in nuclear reactors with neutron capture, partially relies on the availability of isotopically pure target material. For example, the production of the medical radioisotope Lutetium-177, a rising star in nuclear medicine, depends upon the availability of Ytterbium-176 as target material (natural abundance 13%). Similarly, isotopes of Calcium ($Z=20$) and Titanium ($Z=22$) are promising for the production of the medically relevant isotopes Scandium-43, Scandium-44 and Scandium-47. However, both elements have a fragmented natural distribution across 6, respectively 5, stable isotopes. Moreover, Calcium-48 (natural abundance 0.185%) is the most neutron-rich stable isotope that can be used as a beam to synthesize superheavy elements.

Within PRISMAP, the European programme for medical radionuclides, we are investigating the possible enrichment of Titanium and Calcium stable isotopes by means of Separation of Isotopes by Laser Assisted Retardation of Condensation (SILARC). Titanium or Calcium-containing molecules are injected in a gas cell containing Argon as a buffer gas and released via a nozzle creating a supersonic jet. The temperature drops to $\sim 15\text{K}$, at which point Argon atoms cluster around the molecules. If an isotopomer can be selectively excited by an infrared laser, the clusterization can be prevented and the molecule experiences a drag force through the jet, physically separating it from the clusters.

As a first step in this development, Density Functional Theory (DFT) calculations have been performed on Titanium-containing molecules, to determine the ground-state configuration of the molecules (geometry and spin state), their interaction with Ar, and to calculate the frequencies of their vibrational modes. Isotope-selective transitions were identified, mostly in the mid-infrared region. In this contribution, the results from those calculations for simple molecules (TiF_x ($x=1-4$), TiH_x ($x=1-4$)) and complex molecules ($\text{Ti}[\text{OEt}]_4$, $\text{Ti}[\text{OPr}]_4$) will be presented. The infrastructure to investigate SILARC of Titanium at CERN and KU Leuven will be introduced.

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