Theorethical thermochemistry of Po interacting with LBE and filter materials

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One of the goals of theoretical condensed matter physics, is to predict properties of materials directly from the fundamental equations of quantum physics. Density Functional Theory (DFT) is a method that comes close to this goal. Many properties of large classes of solids can be predicted by DFT with an accuracy that often rivals with the accuracy achievable by experiments.

Such a computational approach is particularly attractive when the material under study is not easily accessible by experiment. This is the case for the radiotoxic isotopes of Polonium that are formed by neutron irradiation of the LBE coolant in MYRRHA.

In this contribution, we examine two questions that are related to the behavior of Po in MYRRHA, and this by using DFT and other quantumchemical methods:

- When Po is contained in solidified LBE, to which local environments will it migrate preferentially ?
- If Po is in the gas phase in contact with elements as O, H, Pb and Bi, which small Po-containing molecules can be formed ?

Implications of these results for experimental work will be discussed.