Po-containing Molecules in Fusion and Fission Reactors

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Fission and fusion reactors can only play a role in the future energy landscape if they are inherently safe by design. For some reactor concepts, a major remaining issue is the undesired production of radiotoxic ^{210}Po. To filter out the volatile Po species, information on their molecular composition is needed. An experimental characterization is very challenging due to the large required amount of radioactive Po. An alternative quantum chemistry approach was taken to predict the temperature-dependent stability of relevant diatomic Po-containing molecules. Experimental data on lighter analogue molecules was used to establish a well-founded methodology. The relative occurrence of the Po species was estimated in the cover gas of (i) the leadbismuth eutectic coolant in the accelerator-driven MYRRHA fission reactor and (ii) the PbLi eutectic tritium breeder in the DEMO fusion reactor. In both systems, Po is found to occur mainly as PbPo molecules and atomic Po.

This work[1] illustrates how quantum chemistry for molecules can have impact on engineering decisions for large facilities.

References

1. M.A.J. Mertens et al., J. Phys. Chem. Lett. 2019, 10, 11, 2879-2884
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