Nuclear Density Functional Theory

Exploring Fission and the Limits of the Nuclear Landscape

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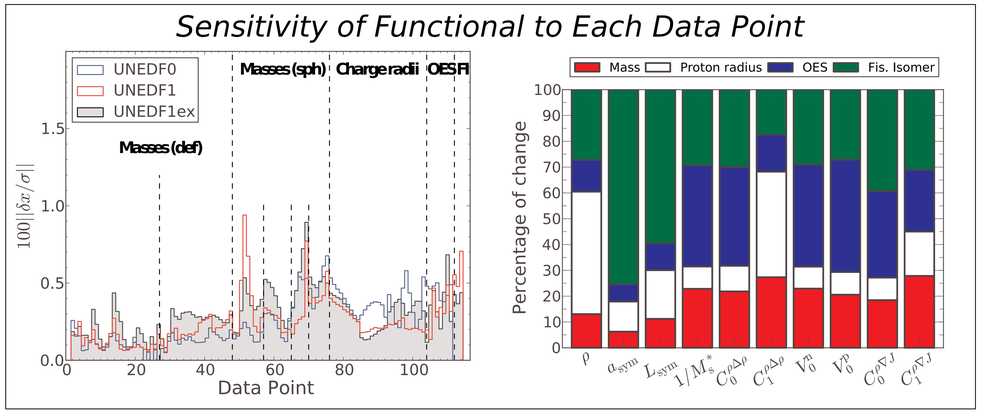
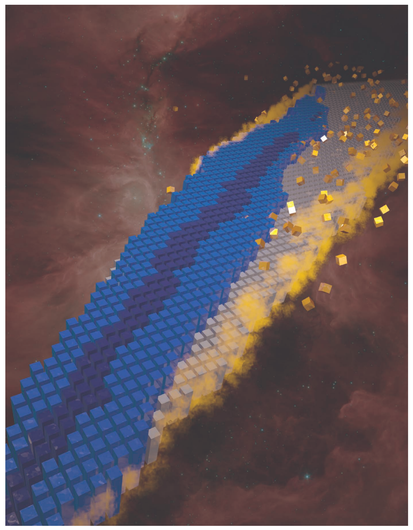
Abstract: We present progress in the construction of a nuclear energy density functional, optimized for deformed nuclei to aid in the study of nuclear fission and nuclei far from stability. We calculate fission barrier heights and spontaneous fission half-lives for even-even actinide nuclei. We also present predictions for the location of the proton and neutron drip lines. Our predictions are found to agree well with empirical data where known, and the consistency between our models lends confidence to our predictions beyond experimentally measured nuclei.

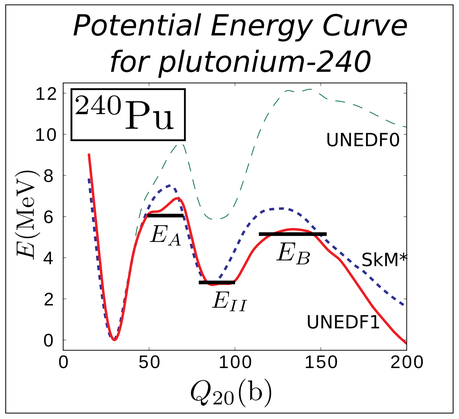
Sensitivity of Functional to Each Data Point



Optimization Methods: A Skyrme-like nuclear energy density functional (EDF) was optimized for masses, radii, and odd-even mass differences for about 80 nuclei across the nuclear chart, including both spherical and deformed nuclei. The optimization was performed through a large-scale least-squares algorithm. The sensitivity of the resulting functional to the selection of data was analyzed...
[M. Kortelainen *et al*, *Phys. Rev.* **C 85**, 024304 (2012)]

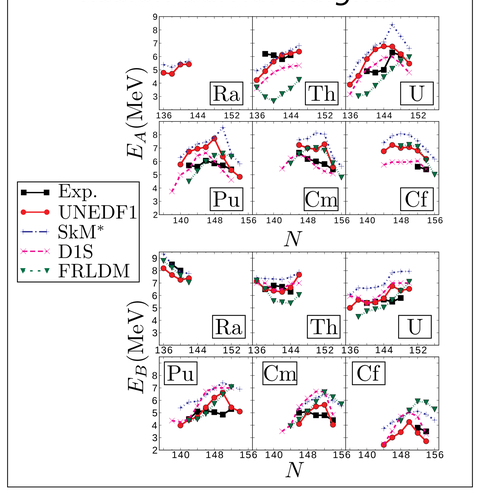


Potential Energy Curve for plutonium-240

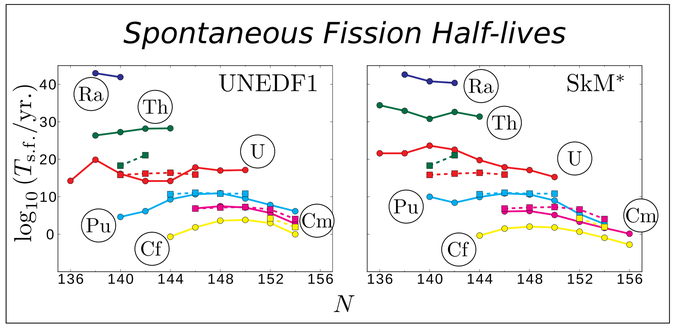


A Functional for Fission: One goal of this program is to obtain a nuclear EDF that is particularly well suited to study nuclear fission. The proper description of fission depends on the ability of the functional to properly describe highly elongated nuclei, and highly elongated nuclei are sensitive to the surface energy predicted by the underlying EDF. It was found through this study that including the fission isomer energies of four nuclei was sufficient to constrain the terms of the functional related to surface energy. With this constraint in place, the UNEDF1 functional predicts fission barrier heights and spontaneous fission half-lives for even-even actinides that are in excellent agreement with empirical values.
[J. McDonnell *et al*, *in preparation*]

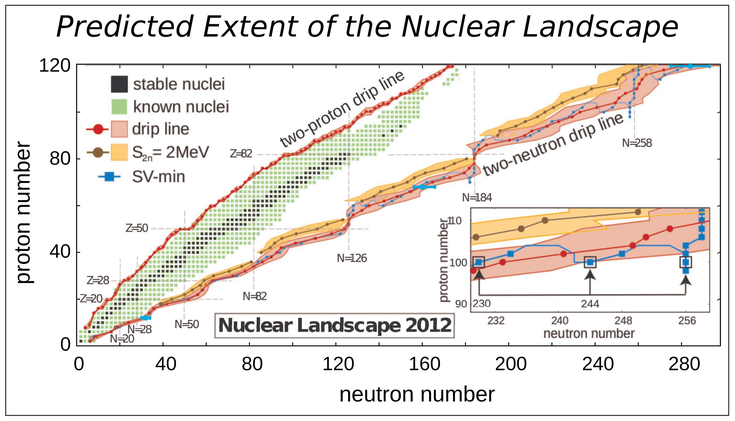
Inner and outer fission barrier heights



Spontaneous Fission Half-lives

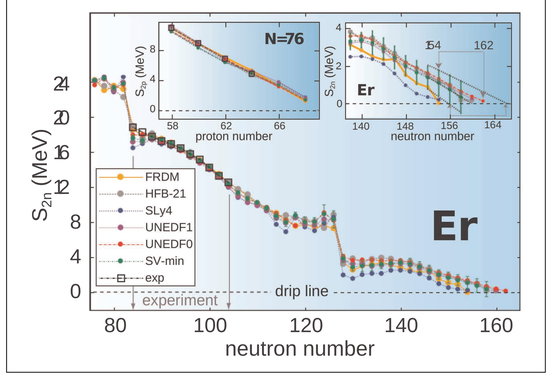


Predicted Extent of the Nuclear Landscape



The Limits of Nuclear Stability: What is the heaviest possible bound nucleus? And how far from stable isotopes do the neutron and proton drip lines extend? And as we calculate the properties of nuclei far from stability, how reliable are our predictions? We can quantify the uncertainty of an EDF both by gauging its sensitivity to the selection of input data and by considering the consistency of the predictions of several theoretical models. While there is a spread in the location where the models predict the drip lines (for example, the predictions for the neutron drip line at erbium extend from N=154 to N=162), the models are nevertheless very consistent with each other over the whole course of the drip lines. Our work in producing the most reliable EDF with controlled uncertainties is expected to lead to predictions that will be valuable for the experiments conducted at facilities such as FRIB and ATLAS.
[J. Erler *et al*, *Nature* **486**, 509-512 (2012)]

Two-Neutron Separation Energy for Erbium



Outlook: Density functional theory, coupled with large-scale computing, has proven to be a powerful tool for nuclear physics theory. The UNEDF1 functional was optimized to capture the essential surface properties for describing aspects of the fission process in even-even actinides. And various EDFs cluster towards predicting the same extent of the nuclear landscape. Future EDFs will be optimized with data that can constrain so far unknown parameters, such as those related to the tensor force. The goal is an EDF of spectroscopic quality with the capability of predicting fission quantities and the properties of exotic nuclei, and NUCLEI is an important step forward.