



Advanced Computational Materials Science: Application to Fusion and Generation-IV Fission Reactors

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An International Workshop Jointly Sponsored by:

Raymond L. Orbach
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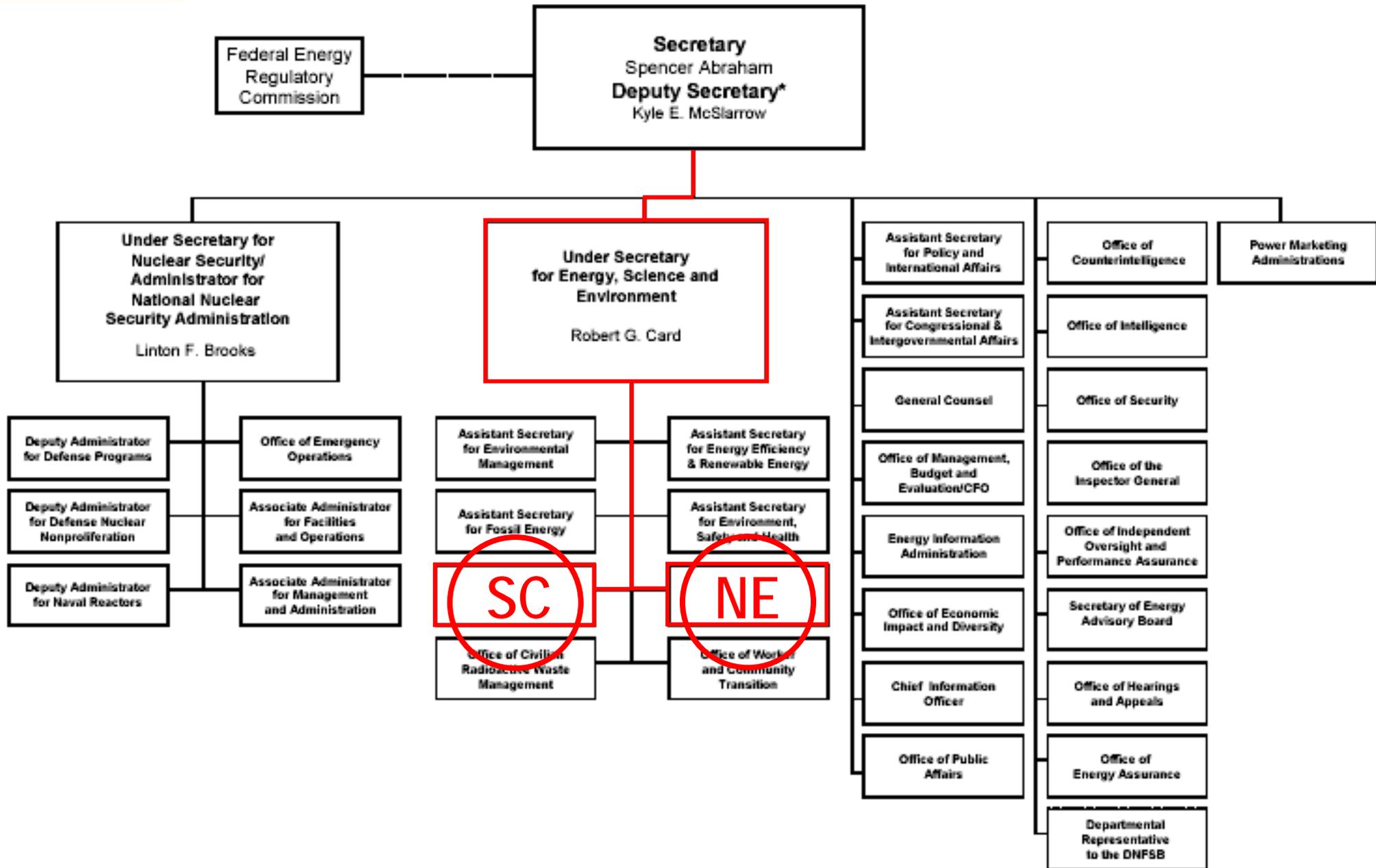
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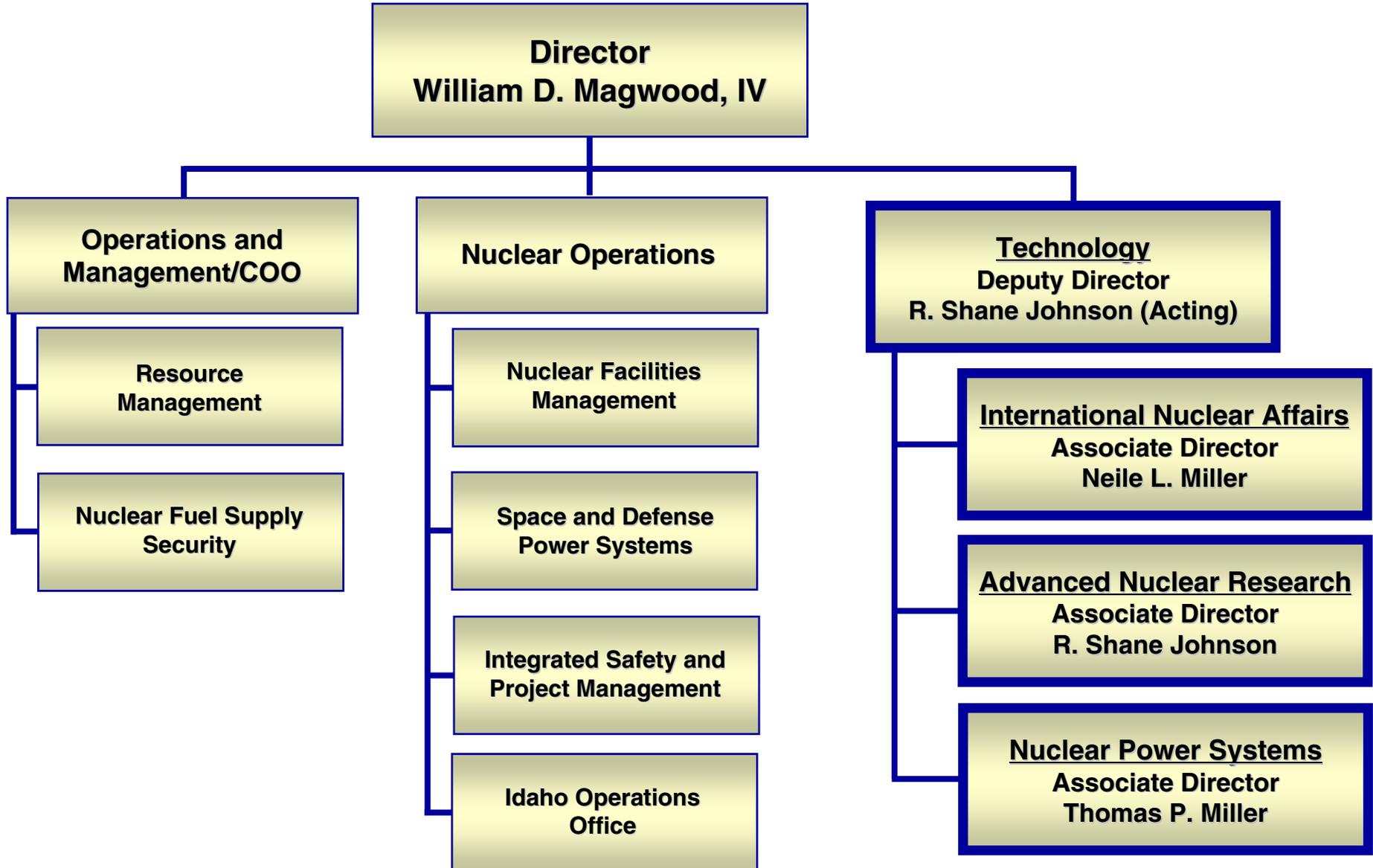
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Purpose

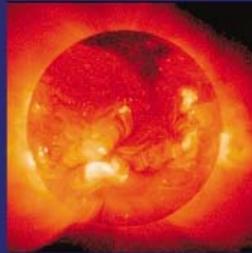
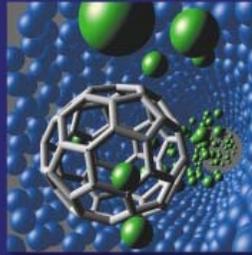
- *Examine the role of high-end computing in the prediction of materials behavior under the full spectrum of radiation, temperature, and mechanical loading conditions anticipated for advanced structural materials that are required for future Generation IV fission and fusion reactor environments*
 - *Evaluate potential for experimentally-validated computational modeling and simulation to bridge the gap between both the available database and what can be obtained in currently-available irradiation facilities, and the ultimate operating environment*
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Timeliness ...

Increased recognition of need for inter-office support to efficiently reach program goals

Office of Science Strategic Plan

February 2004



Office of
Science
U.S. DEPARTMENT OF ENERGY

BES Strategic Timeline

- Complete joint strategic plan and roadmap with the Office of Nuclear Energy (2005)
- Identify key physical processes that help maintain stability of materials during neutron irradiation (2007)
- Complete first draft GEN IV material properties database in support of nuclear power (2010)
- Develop new materials that enable ... breakthroughs for materials in radiation environments, ... (2015)

FES Strategy

- Design ... novel materials ..., leveraging investments through our Fusion Energy Sciences program with the materials research of our Basic Energy Sciences program.

Consider...

- *the topical areas for modeling and simulation, such as microstructural evolution, helium effects, creep rupture, plastic instabilities, and fracture,*
- *computational techniques for spatial and temporal multiscale modeling such as ab initio methods, molecular dynamics, kinetic Monte Carlo, dislocation dynamics, rate theory, micromechanics, and finite element methods,*
- *systems software and tools for high performance computing, such as mathematical software and architecture, languages and compilers, operating systems, computing environments, and visualization, and*
- *adequacy of available neutron source irradiation test facilities, including fission reactors and spallation sources (such as SNS) to provide the experimental data bases for guiding the development of, benchmarking, and validating irradiation response models and simulation tools.*

Goals ...

- *Develop recommendations to ensure that DOE-funded energy research programs can take the fullest possible advantage of future advances in high-end computing, including:*
 - *required software and algorithm development, and their application*
 - *acquisition of and access to high-performance computers*
 - *availability of necessary experimental facilities for validation of theory and modeling*
 - *Provide workshop summary and recommendations to DOE Offices of Science and Nuclear Energy within 60 days (1 June)*
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