

Abstract Submitted
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Opportunities for Computational Discovery in Basic Energy Sciences MARK PEDERSON, Department of Energy, Office of Basic Energy Sciences, Washington DC, 20585-1290 — An overview of the broad-ranging support of computational physics and computational science within the Department of Energy Office of Science will be provided. Computation as the third branch of physics is supported by all six offices (Advanced Scientific Computing, Basic Energy, Biological and Environmental, Fusion Energy, High-Energy Physics, and Nuclear Physics). Support focuses on hardware, software and applications. Most opportunities within the fields of condensed-matter physics, chemical-physics and materials sciences are supported by the Office of Basic Energy Science (BES) or through partnerships between BES and the Office for Advanced Scientific Computing. Activities include radiation sciences, catalysis, combustion, materials in extreme environments, energy-storage materials, light-harvesting and photovoltaics, solid-state lighting and superconductivity. A summary of two recent reports by the computational materials and chemical communities on the role of computation during the next decade will be provided. In addition to materials and chemistry challenges specific to energy sciences, issues identified include a focus on the role of the domain scientist in integrating, expanding and sustaining applications-oriented capabilities on evolving high-performance computing platforms and on the role of computation in accelerating the development of innovative technologies.

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