

Computational Materials Science at the Naval Research Lab: Overview and Some Recent Projects

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Theoretical materials science has been an important part of the Naval Research Laboratory for 50 years. Since then, as computer power increased, the early focus on simple bulk materials has enormously expanded to include complex materials with specific and controllable functionality. New algorithms have also opened the door to studying the complex dynamics of materials at finite temperature far from equilibrium. I will give a brief overview of computational materials science at NRL and illustrate our current interests with several examples from recent projects.