

Abstract Submitted
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Evaluating and enhancing quantum capacitance in graphene-based electrodes from first principles¹ TADASHI OGITSU, Lawrence Livermore National Laboratory, MINORU OTANI, AIST, JONATHAN LEE, MICHAEL BAGGE-HANSEN, JUERGEN BIENER, BRANDON WOOD, Lawrence Livermore National Laboratory — Graphene derivatives are attractive as supercapacitor electrodes because they are lightweight, chemically inert, have high surface area and conductivity, and are stable in electrolyte solutions. Nevertheless, devising reliable strategies for improving energy density relies on an understanding of the specific factors that control electrode performance. We use density-functional theory calculations of pristine and defective graphene to extract quantum capacitance, as well as to identify specific limiting factors. The effect of structural point defects and strain-related morphological changes on the density of states is also evaluated. The results are combined with predicted and measured *in situ* X-ray absorption spectra in order to give insight into the structural and chemical features present in synthesized carbon aerogel samples.

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