

Abstract Submitted
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Center for the Computational Design of Functional Layered Materials: A New Energy Frontier Research Center at Temple University¹
XIAOXING XI, JOHN P. PERDEW, MARIA IAVARONE, XIFAN WU, ADRIENN RUZSINSZKY, JIANWEI SUN, Temple Univ — With Temple as the lead institution, seven universities (including Drexel, Duke, North Carolina State, Pennsylvania, Princeton, and Rice) and one national lab (Brookhaven) have partnered to form a new DOE-supported Energy Frontier Research Center. New or modified materials with desired functionalities play an essential role in the development of clean-energy technologies such as solar cells, batteries, and the generation of hydrogen fuel by water-splitting. Computation of materials properties, based on first-principles theory and modeling, is a promising direction for materials design: quicker and cheaper than experiment, and slower but more reliable than intuition. We aim to design new or defect-modified functional layered materials by theory, modeling, and computation. Candidate materials of special interest will be grown and experimentally characterized in the Center. Detailed experimental and theoretical work will be carried out for catalysis on layered materials, e.g., water splitting. The work of the Center can have important benefits, including new, accurate, and widely useful methods of electronic structure theory, new insights into the materials-by-design problem, and new materials for clean-energy technologies.

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