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**Predicting materials for sustainable energy sources: The key role of density functional theory**

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Climate change and the related need for sustainable energy sources replacing fossil fuels are pressing societal problems. The development of advanced materials is widely recognized as one of the key elements for new technologies that are required to achieve a sustainable environment and provide clean and adequate energy for our planet. We discuss the key role played by Density Functional Theory, and its implementations in high performance computer codes, in understanding, predicting and designing materials for energy applications.