

1. Record Nr.	UNINA9910863176203321
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Titolo	Atomic-Scale Insights into Emergent Photovoltaic Absorbers // by Alex Ganose
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2020
ISBN	3-030-55708-1
Edizione	[1st ed. 2020.]
Descrizione fisica	1 online resource (172 pages)
Collana	Springer Theses, Recognizing Outstanding Ph.D. Research, , 2190-5061
Disciplina	621.31244
Soggetti	Chemistry, Physical and theoretical Renewable energy sources Chemistry, Inorganic Materials Catalysis Force and energy Theoretical Chemistry Renewable Energy Inorganic Chemistry Materials for Energy and Catalysis Physical Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part 1: Introduction -- Chapter 1. Photovoltaics -- Chapter 2. Computational Theory -- Chapter 3. Computational Methodology -- Part 2: Perovskite-Inspired Absorbers -- Chapter 4. Review: Perovskite Photovoltaics -- Chapter 5. Pseudohalide Perovskite Absorbers -- Chapter 6. Vacancy-ordered Double Perovskites -- Part 3. Bismuth-based Absorbers -- Chapter 7. Review: Bismuth-based Photovoltaics -- Chapter 8. Bismuth Chalciodides.
Sommario/riassunto	This book presents an original investigation into alternative photovoltaic absorbers. Solar power is a highly promising renewable energy solution; however, its success is hampered by the limited cost-effectiveness of current devices. The book assesses the photovoltaic

performance of over 20 materials using state-of-the-art, first-principles methods. Adopting a computational approach, it investigates atomic-scale properties at a level of accuracy that is difficult to achieve using laboratory-based experimental techniques. Unlike many theoretical studies, it provides specific advice to those involved in experimental investigations. Further, it proposes directions for future research. This book advances the field of photovoltaics in three crucial ways: firstly, it identifies why one class of proposed materials cannot achieve high efficiency, while at the same time gaining insights that can be used to design future absorbers. Secondly, it shows that poor performance in the bismuth chalcogenides is not due to fundamental limitations, and can be overcome by finely controlling synthesis conditions. Lastly, it describes a range of new stable materials that are expected to show excellent photovoltaic performance. .

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