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	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 Chalcoiodides.
	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 chalcohalides 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. .