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|-------------------------|-------------------------------------------------------------|
| 1. Record Nr.           | UNICAMPANIAVAN0037007                                       |
| Autore                  | Conlon, Lawrence                                            |
| Titolo                  | Differentiable manifolds : a first course / Lawrence Conlon |
| Pubbl/distr/stampa      | Boston, : Birkhäuser, 1993                                  |
| Titolo uniforme         | Differentiable manifolds                                    |
| ISBN                    | 08-17-63626-9                                               |
| Descrizione fisica      | XII, 395 p. ; 25 cm                                         |
| Lingua di pubblicazione | Inglese                                                     |
| Formato                 | Materiale a stampa                                          |
| Livello bibliografico   | Monografia                                                  |
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| 2. Record Nr.           | UNINA9910736031003321                                                                                                                                                                                                                |
| Autore                  | Kamberaj Hiqmet                                                                                                                                                                                                                      |
| Titolo                  | Computer Simulations in Molecular Biology / / Hiqmet Kamberaj                                                                                                                                                                        |
| Pubbl/distr/stampa      | Cham, Switzerland : , : Springer Nature Switzerland AG, , [2023]<br>©2023                                                                                                                                                            |
| ISBN                    | 3-031-34839-7                                                                                                                                                                                                                        |
| Edizione                | [First edition.]                                                                                                                                                                                                                     |
| Descrizione fisica      | 1 online resource (XIII, 298 p. 122 illus., 102 illus. in color.)                                                                                                                                                                    |
| Collana                 | Scientific Computation Series                                                                                                                                                                                                        |
| Disciplina              | 572.80285                                                                                                                                                                                                                            |
| Soggetti                | Molecular biology - Computer simulation<br>Quantum theory - Computer simulation                                                                                                                                                      |
| Lingua di pubblicazione | Inglese                                                                                                                                                                                                                              |
| Formato                 | Materiale a stampa                                                                                                                                                                                                                   |
| Livello bibliografico   | Monografia                                                                                                                                                                                                                           |
| Nota di bibliografia    | Includes bibliographical references and index.                                                                                                                                                                                       |
| Nota di contenuto       | Quantum Mechanics Molecular Dynamics in Simulations -- Basis Set Functions -- Semi-Empirical Quantum Mechanics Molecular Dynamics -- Machine Learning Quantum Mechanics Molecular Dynamics -- Quantum Mechanics Simulations Package. |
| Sommario/riassunto      | This book covers a range of topics in quantum mechanics and                                                                                                                                                                          |

molecular dynamics simulation, including computational modeling and machine learning approaches. The book also provides a Python GUI and tutorials for simulating molecular biological systems and presents case studies of quantum mechanics simulations for predicting electronic properties. Its pedagogical formatting makes it easy for students to understand and follow and has been praised for providing clear and detailed explanations of complex topics. This book is ideal for graduate students and researchers in theoretical and computational biophysics, physics, chemistry, and materials science, as well as postgraduates in applied mathematics, computer science, and bioinformatics.

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