1. Record Nr. UNINA9910814770503321 Autore Micha David A. Titolo Molecular interactions: concepts and methods / / David A. Micha Pubbl/distr/stampa Hoboken, NJ:,: Wiley,, 2020 **ISBN** 1-119-31907-2 1-119-31902-1 1-119-31908-0 Descrizione fisica 1 online resource (402 pages) Disciplina 541.226 Intermolecular forces Soggetti Molecular dynamics Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Sommario/riassunto "Chapters in this book begin with coverage of the concepts and methods for simpler systems, then move on to more advanced subjects for complex systems. Each chapter begins with qualitative aspects before these are treated in quantitative fashion. The first four chapters include the established concepts and quantitative aspects of longrange (electrostatic, induction and dispersion) forces and how they extend to intermediate and short ranges, for ground and excited states. They are followed by chapters dealing with recent developments including electronically non-adiabatic interactions, correlated manyelectron treatments, generalized density functional theory, decomposition and embedding of molecular fragments for large systems, and very recent developments using artificial intelligence with

network training for many-atom systems"--