1. Record Nr. UNINA9910557635903321 Autore Steinbach Martin Titolo On the Stability of Objective Structures / Martin Steinbach . Volume 38 Pubbl/distr/stampa Berlin, : Logos Verlag Berlin, 2021 [s.l.]:,: Logos Verlag Berlin,, 2021 Descrizione fisica 1 online resource (174 p.) Collana Augsburger Schriften zur Mathematik, Physik und Informatik Soggetti Science / Physics Mathematics Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia The main focus of this thesis is the discussion of stability of an Sommario/riassunto objective (atomic) structure consisting of single atoms which interact via a potential. We define atomistic stability using a second derivative test. More precisely, atomistic stability is equivalent to a vanishing first derivative of the configurational energy (at the corresponding point) and the coerciveness of the second derivative of the configurational energy with respect to an appropriate semi-norm. Atomistic stability of a lattice is well understood, see, e.,g., [40]. The aim of this thesis is to generalize the theory to objective structures. In particular, we first investigate discrete subgroups of the Euclidean group, then define an appropriate seminorm and the atomistic stability for a given objective structure, and finally provide an efficient algorithm to check its atomistic stability. The algorithm particularly checks the validity of the Cauchy-Born rule for objective structures. To illustrate our results, we

algorithm.

prove numerically the stability of a carbon nanotube by applying the