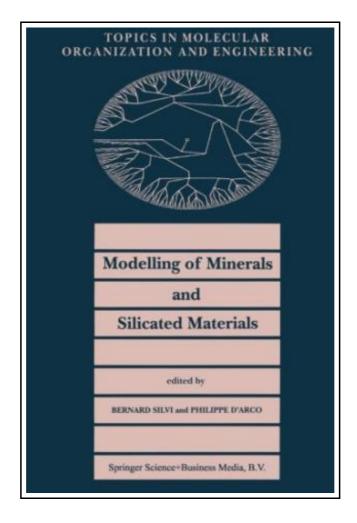
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(Imogene Bergstrom)

MODELLING OF MINERALS AND SILICATED MATERIALS (PAPERBACK)



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Springer, Netherlands, 2013. Paperback. Book Condition: New. 235 x 155 mm. Language: English . Brand New Book ****** Print on Demand ******. The modeling of minerals and silicated materials is a. difficult challenge faced by Solid StatePhysics, Quantum Chemistry and Molecular Dynamics communities. The difficulty of such a modeling is due to the wide diversity of elements, including heavy atoms, and types of bonding involved in such systems. Moreover, one has to consider infinite systems: either perfect cr- tals or glasses and melts. In the solid state a given chemical composition gives rise to numerous polymorphs, geometricallycloselyrelated. These polymorphs have very similar energies and related thermodynamical pr- erties which explain the complexity of their phase diagrams. The modeling of silicates and minerals covers a wide field of applications ranging from basic research to technology, from Solid State Physics to Earth and Planetary science. The use of modeling techniques yields information of different nature. In the case of chemical studies, we can mention inv- tigations on catalytic processes occurring on surfaces and in zeolite cages. These calculations find possible applications in chemical engineering, in particular in the oil industry. Softcover reprint of the original 1st ed. 2002.



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