

Tosi M P. Cohesion of ionic solids in the Born model.  
*Solid State Phys.-Adv. Res. Appl.* 16:1-120, 1964.  
[Argonne National Laboratory, Argonne, IL]

This paper reviews the classical theory of cohesion in ionic crystals, developed in the early decades of this century mainly by Max Born. Advances in the determination of interionic forces, their relation to cohesive properties and ionic radii, and applications to structural phase transitions and surface properties are discussed. [The *SCI*<sup>®</sup> indicates that this paper has been cited in over 465 publications since 1964.]

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"Experimental interest in the properties of lattice defects in ionic materials was very high in the early-1950s. It stimulated our group at the University of Milan, under the leadership of Fausto Fumi, to theoretical work, applying the simple Born model of interionic forces to these problems. This choice of activity for our group, which was beginning its growth in a country emerging from a destructive war and in a national cultural background where solid-state theory was still largely unknown, combined good topical interest with modesty of needs. A subscription to *Physical Review* absorbed a large part of our research budget.

"It soon became clear during our work that one had to go back and reexamine the determination of the inter-

ionic forces. Fausto and I devoted several years to this work in the early-1960s when we were with the Solid State Science Division of Argonne National Laboratory. The atmosphere in the division at that time, under the directorship of Oliver Simpson, was very good; we were encouraged to pursue our interest in giving a new look at a rather old field, although our research could in no way be construed as being either fashionable or applications-oriented. Our essential results were published in two joint papers.<sup>1,2</sup> The main points are the connection between interionic forces and ionic radii and a careful analysis of cohesive data. The review article on cohesion in ionic crystals, whose preparation had actually been brought forward with Fausto at the same time, is the conclusive step of this series of studies on interionic forces.

"Our patient effort has found its main usefulness in a direction that I had not then envisaged. In the 1970s molten salts became a favorite object for computer simulation work and our analysis of interionic forces for these materials in the solid state has been used with some satisfaction by groups engaged in this liquid-state activity. Computer simulation results are confronted in this area<sup>3,4</sup> by a vast amount of experimental data, both of a traditional type (thermodynamic and transport properties) and of a modern type (neutron diffraction and inelastic scattering). My review article seems to have become a rather standard reference to the basic model underlying the physics of simple ionic materials."

1. Fumi F G & Tosi M P. Ionic sizes and Born repulsive parameters in the NaCl-type alkali halides—I. The Huggins-Mayer and Pauling forms. *J. Phys. Chem. Solids* 25:31-43, 1964.  
[The *SCI* indicates that this paper has been cited in over 195 publications since 1964.]
2. Tosi M P & Fumi F G. Ionic sizes and Born repulsive parameters in the NaCl-type alkali halides—II. The generalized Huggins-Mayer form. *J. Phys. Chem. Solids* 25:45-52, 1964.  
[The *SCI* indicates that this paper has been cited in over 175 publications since 1964.]
3. Sangster M J L & Dixon M. Interionic potentials in alkali halides and their use in simulations of the molten salts. *Advan. Phys.* 25:247-342, 1976.
4. Parrinello M & Tosi M P. Structure and dynamics of simple ionic liquids. *Riv. Nuovo Cimento* 2:1-69, 1979.