

**Prof. Alexander Shlyuger**

**Complete list of published contributions to scientific research**

**Books:**

1. Co-authored book: Kantorovich, L., Kotomin, E., Kuzovkov, V., Tale, I.; Shluger, A. and Zakis, Yu. Models of processes in insulating solids with defects, 1991, (Riga: Zinatne), 350p (in Russian).
2. Co-edited book: Quantum Mechanical Cluster Calculations in Solid State Studies, Edited by R. W. Grimes, C. R. A. Catlow, and A. L. Shluger, 1991, (World Scientific: Singapore), 470 p.

**Books chapters:**

1. Zhidomirov, G. M.; Shluger, A. L.; Kantorovich, L. N., Theoretical models in chemisorption theory. In: *Problems of Quantum Chemistry* (Leningrad: Nauka), v. 2, 1987, pp.225-275 (in Russian).
2. Shluger, A. L., Rohl, A. L., Gay, D. H., and Williams, R. T., Theory of the Interaction between AFM tips and Ionic Surfaces, in: "Forces in Scanning Probe Microscopy", Eds. H. -J. Güntherodt, D. Anselmetti, E. Mayer, NATO ASI Series E: Applied Sciences, v. **286**, 1995, pp. 169 - 174.
3. Shluger, A. L. Theoretical Studies of the Models of Self-Trapped Excitons and Holes in Ionic Crystals, in: *Relaxations of Excited States and Photo-Induced Phase Transitions*, Ed. K. Nasu (Springer: Berlin, 1997), pp. 203 - 211.
4. Shluger, A. L., Foster, A. S., C. Barh and M. Reichling, Contrast mechanisms in NC-AFM on ionic surfaces. - In: *Non-Contact Atomic Force Microscopy*, (Springer, Nanoscience and Technology series), Edited by S. Morita, R. Wiessendanger, E. Meyer, 2002, pp. 305-348.
5. Stoneham A. M., Shluger A. L., Foster A. S., and Szymanski M. A., Defects and Defect-controlled Behaviour in High-k Materials: a Theoretical Perspective, - In: *High-k gate dielectrics*, Ed.: M. Housa, IOP, 2003, pp. 293 – 324.
6. Shluger A. L., Foster A. S., Gavartin J., and Sushko P. V., Defects in wide-gap oxides: Computer modelling and challenges, - In: *Nano and Giga Challenges in Microelectronics*, Eds.: J. Greer, A. Korkin, J. Lobanowski, pp. 151-222, ISBN: 0-444-51494-5, Elsevier 2003.
7. Stoneham A. M. and Shluger A. L., Electronic Structure: Impurity and Defect States in Insulators, In: *Encyclopedia of Condensed Matter Physics*, Eds.: F. Bassani, J. Leidl, and P. Wyder, Elsevier, 2005

### Review articles:

1. Shluger, A. L.; Harker, A. H.; Grimes, R. W. and Catlow, C. R. A. Crystal excitation: Survey of many-electron Hartree-Fock calculations of self-trapped excitons in insulating crystals. - *Phil. Trans. Royal Society London A*, 1992, v. **341**, p. 221-231.
2. \*Shluger, A. L. and Stoneham A. M. Small Polarons in Real Systems: Concepts and Problems. - *J. Phys.: Condensed Matter*, 1993 , v. **5**, Nr. 19, 3049-3086.
3. Shluger, A. L. and Rohl, A. L., A Model of Interaction of Ionic Tips with Ionic Surfaces for Interpretation of Scanning Force Microscope Images. - *Topics in Catalysis* 1996, v. **3**, No. 1,2, p. 221-248.
4. Shluger, A. L., Livshits, A. I., Foster, A. S., and Catlow, C. R. A., Models of Image Contrast in Scanning Force Microscopy on Insulators, *J. Phys.: Condensed Matter*, 1999, v. **11**, p. R295 - R322.
5. Shluger, A. L., Gavartin, J. L., Szymanski, M. A., and Stoneham, A. M., Atomistic modelling of radiation effects: towards dynamics of exciton relaxation, *Nucl. Instr. Methods B*, 2000, v. **166-167**, pp. 1-12.
6. \*W. A. Hofer, A. S. Foster, and A. L. Shluger, Theories of Scanning Probe Microscopes at the Atomic Scale, - *Rev. Mod. Phys.* 2003, v. **75**, No 4, pp. 1287 - 1331.
7. \*W. P. Hess, A. G. Joly, K. M. Beck, M. Henyk, P. V. Sushko, P. E. Trevisanutto, and A. L. Shluger. "Laser control of desorption through selective surface excitation", - *J. Phys. Chem. B* feature article – 2005, v. **109**, No 43, pp. 19563-19578.

### Research articles:

8. Shluger, A.; Kotomin, E.; Dzelme, Yu. Quantum - chemical calculation of electronic and hole centres and surface of NaCl crystals (I). - *Phys. State. Sol. (b)*, 1979, v. **96**, Nr. 1, p. 91-99.
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10. Shluger, A. L.; Kotomin, E. A. Semiempirical calculations of defect properties in LiF crystal. I. Perfect crystal. - *Phys. Stat. Sol. (b)*, 1981, v. **108**, Nr.2., p.673-681.
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12. Kotomin, E. A.; Shluger, A. L. Quantum - chemical simulation of Frenkel-pair separation in LiF crystals. - *Solid State Commun.*, 1981, v. 40, Nr. 4, p. 665-673.
13. Shluger, A.; Kotomin, E. and Kantorovich, L. Calculation of energies of radiative tunneling transitions between defects in alkali halides. - *Solid State Commun.*, 1982, v. **42**, Nr.10, p. 749-752.
14. Ermoshkin, A. N.; Kotomin, E. A.; Shluger, A. L. The semi-empirical approach to electronic structure of ionic crystal surface. - *J.Phys.C: Solid State Phys.*,1982, v.**15**, p. 847-861.
15. Ivanov, G. K.; Kozhushner, M. A.; Shluger, A. L. The mechanism and kinetics of radiative - tunnelling transitions. - *Chemical Physics* (Russian), 1982, Nr. 7, p. 907-914.
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17. Kantorovich, L. N., Shluger, A. L. Adsorption of the water molecule on alkali-halide crystal surface. - *Chemical Physics* (Russian), 1982, Nr. 10, p. 1341- 1348.
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19. Kantorovich, L. N.; Shluger, A. L.; Tiliks, Yu. E. Adsorbed molecules interaction with alkali - halides crystals surfaces. - *Chemical Physics* (Russian), 1984. v. **3**, Nr. 6, pp. 894-899.
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23. Shluger, A. On the non-equivalence of Si-O bonds in silicon dioxide. - *J. Phys. Chem. Solids.* 1986, v. **47**, Nr. 7, p. 659-664.
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## **Patents**

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