Dr. Anton Vasyunin
Curriculum Vitae

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1. Date of Birth: February 11, 1983
2. Citizenship: Russian
3. Employment:
   (1) 07/2014 - present; Max-Plank-Institute for Extraterrestrial Physics, Garching, Germany
   (2) 10/2013 - 06/2014; University of Leeds, School of Physics and Astronomy, Research Associate
   (3) 09/2010 - 09/2013; first at The Ohio State University, now at the University of Virginia (moved with the group in Sep. 2011), Research Associate, Group of Professor Eric Herbst
   (4) 12/2009 - 08/2010: The Max Planck Institute for Astronomy, Postdoctoral Fellow Department of Planet and Star Formation; head: Professor Thomas Henning
4. Education:
   (1) University of Heidelberg, Max-Planck-Institute for Astronomy (Germany), Dr. rer. nat. (PhD), graduated on December 2, 2009. Thesis title: "Chemistry in the ISM and disks on the verge of planet formation". Supervisors: Dr. Dmitry Semenov, Prof. Dr. Thomas Henning.
   (2) Ural State University, Ekaterinburg (Russia), Master of Physics, graduated in 2005. Thesis title: "The modification of Monte Carlo technique for the modeling of interstellar chemistry". Supervisor: Dr. Andrej Sobolev.
   (3) Ural State University, Ekaterinburg (Russia), Bachelor of Physics, graduated in 2003. The title of thesis: "Modeling of methanol evaporation in a shock wave". Supervisor: Dr. Andrej Sobolev.
   (4) High school 66 with advanced training in mathematics and physics, Ekaterinburg (Russia), graduated in 1999 with distinction (gold medal for excellent study).
5. Research interests:
   (1) Mathematical methods of astrochemical modeling. Development and incorporation of stochastic approaches to grain surface chemistry in gas-grain chemical models with many gas-phase and surface reactions. Detailed modeling of the structure of layered icy grain mantles with a macroscopic Monte Carlo approach.
   (2) Observational manifestations of grain surface chemistry in various astrophysical environments: complex organic molecules in the cold ISM at 10 K, chemistry of infrared dark clouds, complex organic chemistry during the warm-up stage of hot core formation.
   (3) Chemical evolution of protoplanetary disks with inclusion of grain evolution. Interplay among chemistry, physical structure, and dynamics of disks. Formation of complex molecules in disks.
   (4) Uncertainties in astrochemical modeling. Identification of most "uncertain" important chemical processes for further laboratory studies.
6. Scholarships and Honours:
   (1) Sverdlovsk region Governor's prize (2007)

(2) Prize of Dynasty foundation (2005, 2006, 2007)
(3) INTAS PhD fellowship (2006, cancelled due to move to Heidelberg)
(4) 2nd prize winner, Russian competition of the best Master theses in physics (2005)
(5) 3d prize winner, competition of student research talks (more than 20 talks), Russian student conference "Physics of Space" (2004)
(6) K.A. Barkhatova's scholarship of Physical Department of the Ural State University for the best students in astronomy (2003)
(7) A.S. Popov scholarship for the best students in physics by the Ural Museum of Radio (2002)
(8) 2nd prize winner, All-Russian competition of students investigations "Astronet-2002" (2002)
(9) 1st prize winner, competition of student research talks (more than 20 talks), Russian student conference "Physics of Space" (2001, 2002)

7. Important oral presentations:

(1) Stochastic and deterministic approaches to model grain-surface chemistry // COSPAR 2014, Moscow, Russia
(2) New chemical models for new era observations: a multiphase Monte Carlo model of gas-grain chemistry // The Molecular Universe, 280th Symposium of the International Astronomical Union held in Toledo, Spain, May 30-June 3, 2011

8. Observational experience:

(1) The Onsala 20m proposal "Class II methanol maser sources at 37.7 GHz". PI: A.I. Vasyunin (2005)
(2) Two summer projects in Puschino radioastronomy observatory (Russia) in 2000 and 2001: searching for methanol maser emission at 34.5 GHz and 37.7 GHz

9. Journal referee

(1) Astronomy & Astrophysics, The Astrophysical Journal, The Astrophysical Journal Letters

10. Summer schools:

(1) 38th Saas Fee Winter school "Millimeter Astronomy", March 3—8 2008, Les Diablerets, Switzerland
(2) VLTI summer school "Circumstellar disks at very high angular resolution", May 28 — June 8 2007, Porto, Portugal
(3) Young radioastronomers' school, Puschino, Russia (2001)
(4) "Physics of Space", Yekaterinburg, Russia (2000—2008, 2010, 2012)

11. Computer skills:

(1) Windows (expert knowledge), Linux (advanced user)
(2) Fortran, IDL, Axum, Gildas, XS, TeX
(3) SQL (MySQL), PHP/HTML/CSS
(4) Complete cycle of website development including SEO skills

12. Languages:

(1) Russian (mother tongue)
(2) English (fluent)
(3) German (basic)

13. Refereed papers (published):

(1) *D.M. Graninger, E. Herbst, K.I. berg,* ***A.I. Vasyunin*** The HNC/HCN Ratio in Star-forming Regions // The Astrophysical Journal, Volume 787, Issue 1, article id. 74, 11 pp. (2014)

(2) *A. Occhiogrosso, **A.I. Vasyunin**, E. Herbst, S. Viti, M.D. Ward, S.D. Price, W.A. Brown* Ethylene oxide and acetaldehyde in hot cores // Astronomy & Astrophysics, Volume 564, id.A123, 9 pp. (2014)

(3) *C. Walsh, T.J. Millar, H. Nomura, E. Herbst, S. Widicus Weaver, Y. Aikawa, J.C. Laas, **A.I. Vasyunin*** Complex organic molecules in protoplanetary disks // Astronomy & Astrophysics, Volume 563, id.A33, 35 pp. (2014)

(4) *T. Vasyunina, **A.I. Vasyunin**, E. Herbst, H. Linz, M. Voronkov, T. Britton, I. Zinchenko, F. Schuller* Organic Species in Infrared Dark Clouds // The Astrophysical Journal, Volume 780, Issue 1, article id. 85, 19 pp. (2014)

(5) *O.V. Kochina, D.S. Wiebe, S.V. Kalenskii, **A.I. Vasyunin*** Modeling of formation of complex molecules in protostellar objects // Astronomy Reports, Volume 57, Issue 11, pp. 818–832 (2013)

(6) *T. Albertsson, D.A. Semenov, **A.I. Vasyunin**, T. Henning, E. Herbst* New extended deuterium fractionation model: assessment at dense ISM conditions and sensitivity analysis // ApJS, Volume 207, Issue 2, article id. 27, 29 pp. (2013)

(7) ***A.I. Vasyunin**, E. Herbst* Reactive desorption and radiative association as possible drivers of complex molecule formation in the cold interstellar medium // ApJ, Volume 769, Issue 1, article id. 34, 9 pp. (2013)

(8) *V. Akimkin, S. Zhukovska, D. Wiebe, D. Semenov, Ya. Pavlyuchenkov, **A.I. Vasyunin**, T. Birnstiel, T. Henning* Protoplanetary disk structure with grain evolution: The ANDES model // ApJ Volume 766, 8 (2013)

(9) ***A.I. Vasyunin**, E. Herbst* A Unified Monte Carlo Treatment of Gas-Grain Chemistry for Large Reaction Networks. II. A Multiphase Gas-surface-layered Bulk Model // ApJ, Volume 762, Issue 2, article id. 86, 21 pp. (2013)

(10) *T. Vasyunina, **A.I. Vasyunin**, E. Herbst, H. Linz* Chemical Modeling of Infrared Dark Clouds: The Role of Surface Chemistry // ApJ, Volume 751, Issue 2, article id. 105, 12 pp. (2012)

(11) *D.A. Neufeld, E. Falgarone, M. Gerin, B. Godard, E. Herbst, G. Pineau des Forêts, **A.I. Vasyunin**, R. Güsten, H. Wiesemeyer, O. Ricken* Discovery of interstellar mercapto radicals (SH) with the GREAT instrument on SOFIA // A&A, Volume 542, id.L6, 4 pp. (2012)

(12) *V.V. Akimkin, Y.N. Pavlyuchenkov, **A.I. Vasyunin**, D.S. Wiebe, M.S. Kirsanova, T. Henning* UV-controlled physical and chemical structure of protoplanetary disks // Astrophysics and Space Science, DOI: 10.1007/s10509-011-0652-7 (2011)

(13) ***A.I. Vasyunin**, D.S. Wiebe, T. Birnstiel, S. Zhukovska, T. Henning, C.P. Dullemond* Impact of Grain Evolution on the Chemical Structure of Protoplanetary Disks // ApJ, Vol. 727 issue 2 (2011)

(14) *R. Garrod, **A.I. Vasyunin**, D.A. Semenov, D.S. Wiebe, Th. Henning* A new modified-rate approach for gas-grain chemistry: Comparison with a unified large-scale Monte Carlo simulation // ApJL, Vol. 700 issue 1, pp. L43-L46 (2009)

(15) ***A.I. Vasyunin**, D.A. Semenov, D.S. Wiebe, Th. Henning* A Unified Monte Carlo Treatment of Gas-Grain Chemistry for Large Reaction Networks. I. Testing Validity of Rate Equations in Molecular Clouds // ApJ, Vol. 691, 1459V (2009)

(16) ***A.I. Vasyunin**, D.A. Semenov, Th. Henning, Wakelam, V., Herbst, E., A.M. Sobolev* Chemistry in Disks: A Sensitivity Analysis // ApJ, Vol. 672, 629V (2008)

(17) ***A.I. Vasyunin**, A.M. Sobolev, D.Z. Wiebe, D.A. Semenov* Influence of Uncertainties in the Rate Constants of Chemical Reactions on Astrochemical Modeling Results // Astronomy Letters, Vol. 30, Issue 8, p.566-576

14. Conference proceedings:

(1) *A.I. Vasyunin* Interstellar Ices: Invited lecture for students // Physics of Space: the 41st Annual Student Scientific Conference. Published by The Ural Federal University, 2012, pp.19-42.

(2) *A.I. Vasyunin; E. Herbst* Monte Carlo Modeling of Gas-Grain Chemistry in Star-Forming Regions // International Symposium On Molecular Spectroscopy, 66th Meeting, Held 20-24 June, 2011 at Ohio State University

(3) *A.I. Vasyunin; E. Herbst* New chemical models for new era observations: a multiphase Monte Carlo model of gas-grain chemistry // The Molecular Universe, Proceedings of the 280th Symposium of the International Astronomical Union held in Toledo, Spain, May 30-June 3, (2011)

(4) *R. Garrod; A.I. Vasyunin* New Methods for Interstellar Grain-Surface Chemistry Simulations: A New Modified-Rate Approach. // Bulletin of the American Astronomical Society, Vol. 41, p.836 (2010)

(5) *Vasyunin, A. I.; Semenov, D.; Henning, Th.; Wakelam, V.; Herbst, E.; Sobolev, A. M.* Chemistry in Protoplanetary Disks: Analysis of uncertainties. // Conference proceedings: Molecules in Space and Laboratory, Paris, 14-18 May, 2007.

(6) *A.I. Vasyunin, D.A. Semenov, A.M. Sobolev, Th. Henning* Reliability of disk chemical modelling. // "Science with ALMA: a new era for Astrophysics" International Conference,13 - 17 November 2006, Madrid, Spain, p.88.

(7) *A.I. Vasyunin, D.A. Semenov, A.M. Sobolev, Th. Henning* Reliability of disk chemical modelling. // Proceedings of symposium "Complex molecules in Space: Present status and prospects with ALMA", May 8-May 11, 2006, Fuglsocentret, Denmark, p.68

(8) *A.I. Vasyunin* Stochastic modelling of chemical evolution of interstellar meidum with gas-grain interaction. // Proceedings of symposium "Star formation in Galaxy and outside", Apr.17-Apr.18, 2006, Moscow, Janus-K, 2006, pp.119-125

(9) *Sobolev A.M., Vasyunin A.I.* Quantification of uncertainties in the model interstellar chemical abundances arising from inaccuracies in reaction rates. In: The Dense Interstellar Medium in Galaxies, 4th Cologne-Bonn-Zermatt-Symposium, held in Zermatt, Switzerland, September 22-26, 2003, Abstract book, 2003, p.282

Anton I. Vasyunin
Abstract of Current Research

1 Motivation

The area of my major scientific interests is the chemical complexity of star- and planet-forming regions. I approach research problems in this area by constructing sophisticated numerical models. Models help us to examine chemical principles discovered on Earth in extreme conditions of interstellar medium (ISM), understand observations, and ultimately answer the question of whether it is possible to form complex prebiotic molecules in space.

Formation and destruction of molecules in the interstellar medium occurs in chemical reactions both in the gas phase and on surfaces of tiny interstellar grains. While the majority of simple observed molecules are formed in ion-molecular gas phase reactions, the chemistry on grain surfaces appears to play a key role both in the formation of the simplest molecule H_2, which initiates ion-molecular chemistry, and in the assembly of complex organic species — possible precursors of life. Certain organic molecules of terrestrial type such as methanol, methyl formate, and dimethyl ether were discovered in star-forming regions a while ago. Correspondingly, the first relatively simple models of interstellar gas-grain chemistry were developed more than twenty years ago (e.g, Hasegawa et al. (1992)). These models (both their mathematical formalism and, to a lesser degree, their networks of surface chemical reactions) were used almost unchanged over the last twenty years. Although results produced with these models are still satisfactory to explain observational data in many cases, rapid progress in laboratory and observational astrophysics dictates the need for development of new advanced models of gas-grain chemistry, with an emphasis on a more accurate treatment of grain-surface chemistry and the chemistry of complex organic species.

2 Ongoing research

The macroscopic Monte Carlo algorithm for the simulation of chemically reactive systems is a most most promising technique, which makes it possible to combine an advanced approach to grain-surface chemistry with a full-scale chemical network (hundreds of species, thousands of reactions). I was the first to construct a full-scale model of the chemical evolution of the interstellar medium in which gas-phase and grain surface chemistry are treated simultaneously with a Monte Carlo approach [2]. With this model, I investigated the importance of the discreteness of surface reactions for the chemical evolution of molecular clouds, and tested the validity of the new approximate modified rate equation (MRE) method proposed in [12]. It was confirmed that the new MRE approach gives more accurate results for grain-surface chemistry than normal rate equations [4].

Recently, the macroscopic Monte Carlo model of gas-grain chemistry was extended to take into account the multilayer nature of icy grain mantles and incorporate laboratory data on ice desorption correctly [7]. The ice treatment includes a distinction between a reactive ice surface and an inert bulk. The treatment also distinguishes between zeroth- and first-order desorption, and includes the entrapment of volatile species in more refractory ice mantles. We applied the model to the investigation of the chemistry in hot cores, in which a thick ice mantle built up during a previous cold phase of protostellar evolution undergoes radical-radical surface reactions during warm-up and is eventually evaporated. For the first time, the impact of a detailed multilayer approach to grain mantle formation on the warm-up chemistry is explored. The use of a multilayer ice structure has a mixed impact on the abundances of organic species formed during the warm-up phase. For example, the abundance of gaseous $HCOOCH_3$ is lower in the multilayer model than in previous grain models, which do not distinguish between layers (so-called two phase models). Other gaseous organic species formed in the warm-up phase are affected slightly. Finally, we find that the entrapment of volatile species in water ice can explain the two-jump behavior of H_2CO previously found in observations of protostars. The two-jump behavior cannot be explained with traditional rate equation-based models.

The impact of grain-surface chemistry on the abundances of species in the gas phase was further investigated with rate equation-based models for the case of infrared dark clouds (IRDCs) [5, 6]. IRDCs are considered in the literature as possible earliest stages of massive star formation. In comparison to low-mass starless and prestellar cores, they are characterized by somewhat higher densities (10^5—10^6 cm^{-3} vs. 10^4 cm^{-3}) and elevated temperatures (various estimations give values from 15 K to 30-40 K vs. 10 K). The range of temperatures typical for IRDCs is very promising for investigation of the impact of grain-surface chemistry on the abundances of gas-phase species, since at these temperatures grain-surface chemistry is strongly coupled to gas-phase chemistry via fast processes of accretion and desorption. Our study revealed the role of surface chemistry in explaining the systematically higher abundance of N_2H^+ in IRDCs compared with colder low-mass prestellar cores and warmer high-mass protostellar objects (HMPOs). The chemical reason is that at 20 K–30 K the precursor of N_2H^+, the N_2 molecule, does not freeze out onto grains, but also is not efficiently destroyed in reactions with CO, because at this temperature the carbon monoxide abundance in the gas is reduced. The reason for this reduction is that CO at 20 K–30 K is converted by grain-surface reactions to CO_2 and other molecules more rapidly, which then desorb back into the gas phase.

The recent discovery of complex organic molecules (COMs) in cold prestellar clouds at 10 K [10, 11] gave another opportunity to investigate the impact of grain-surface chemistry on the molecular inventory of interstellar gas. The abundances of these molecules cannot be explained by the previously developed "warm-up" scenario, in which organic molecules are formed via diffusive chemistry on surfaces of interstellar grains starting at 30-40 K, and then released to the gas at higher temperatures during later stages of star formation. In a recently submitted article [8], we investigated an alternative scenario in which organic species are formed via a sequence of gas-phase reactions between simple species formed on grain surfaces and then ejected into the gas via efficient reactive desorption, a process in which non-thermal desorption occurs as a result of conversion of the exothermicity of chemical reactions into the ejection of products from the surface. The proposed scenario leads to reasonable results at temperatures as low as 10 K and may be considered as a step towards the explanation of abundances of terrestrial-like organic species observed during the earliest stages of star formation.

Another area of my research interests concerns the chemistry in protoplanetary disks. During my PhD studies, I carried out an investigation of the impact of uncertainties in rate coefficients of chemical reactions on the results of chemical modeling of protoplanetary disks [1]. It was found that for the majority of observationally important species, the calculated uncertainties lie within one order of magnitude with a tendency to increase with the complexity of a molecule. Next, in [3], a gas-grain chemical model was coupled to a sophisticated model of grain coagulation and sedimentation [9] and d'Alessio-like model for the structure of a protoplanetary disk. With this set of models, the impact of grain evolution on the chemical structure of protoplanetary disks was investigated. It was found that the major influence on chemistry comes from the reduced opacity of dust due to sedimentation. Molecular tracers of grain growth were proposed.

3 Future research plans

The sensitivity of modern radio telescopes is constantly improving. Thus, molecules with very low fractional abundances become detectable in the gas phase. The first detection of complex organic species with fractional abundances of $\sim 10^{-11}$ with respect to hydrogen [10, 11] in cold interstellar medium is very promising. Low-abundance COMs may probably serve as sensitive tracers of chemical reactions on grain surfaces and processes of desorption (both thermal and non-thermal). As such, further development of advanced models of grain surface chemistry as parts of gas-grain models and investigation of the impact of grain surface chemistry on the abundances of gas-phase species remains an interesting topic of research for me.

In addition to a detailed treatment of grain surface chemistry, the explanation of the chemistry of low-abundant species requires improvement of networks of gas-phase reactions. Existing networks are designed to reproduce abundances of generally abundant species with fractional abundances $\geq 10^{-9}$ to hydrogen. The chemistry of species with low abundances is incomplete in these networks, because many slow chemical processes such as formation of complex molecular ions by radiative association reactions was not considered carefully before because the products were not detectable. The inclusion of the gas-phase chemistry of complex organic molecules in chemical models is a necessary step towards future models of organic chemistry in regions of star formation.

The angular resolution of new observational facilities such as ALMA will soon reach 1/100 of an arc second. As such, small spatial inhomogeneities in the spatial distribution of molecules in star-forming regions and protoplanetary disks become visible. Because of this advance, I see another research topic of interest: the development of multidimensional hydrodynamical models of the ISM with chemical evolution. Such models will be useful for explanation of the spatial distribution of molecular species, and for better understanding star formation starting from the fragmentation of a giant molecular cloud to the formation of protostars and circumstellar disks. Coupled with realistic chemical models, hydrodynamic models will provide new insight into the evolution of chemical complexity of matter during the fundamental formation of stars and planetary systems.

References

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[2] Vasyunin, A. I., Semenov, D. A., Wiebe, D. S., & Henning, T. 2009, Astrophys. J, 691, 1459

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