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## Publications

### **Elongation mechanism of the ion shaping of embedded gold nanoparticles under swift heavy ion irradiation**

Vu, T. H. Y., Dufour, C., Khomenkov, V., Leino, A. A., Djurabekova, F., Nordlund, K., Coulon, P. -E., Rizza, G. & Hayoun, M., 15 Jul 2019, In : Nuclear Instruments & Methods in Physics Research. Section B: Beam Interactions with Materials and Atoms. 451, p. 42-48 7 p.

### **Cascade overlap with vacancy-type defects in Fe**

Granberg, F., Byggmästar, J. & Nordlund, K., 3 Jul 2019, In : European Physical Journal B. Condensed Matter and Complex Systems. 92, 7, 7 p., 146.

### **Historical review of computer simulation of radiation effects in materials**

Nordlund, K., Jul 2019, In : Journal of Nuclear Materials. 520, p. 273-295 23 p.

### **Collision cascades overlapping with self-interstitial defect clusters in Fe and W**

Byggmästar, J., Granberg, F., Sand, A. E., Pirttikoski, A., Alexander, R., Marinica, M. C. & Nordlund, K., 19 Jun 2019, In : Journal of Physics. Condensed Matter. 31, 24, 15 p., 245402.

### **Channeling maps for Si ions in Si: Assessing the binary collision approximation**

Hobler, G. & Nordlund, K., 15 Jun 2019, In : Nuclear Instruments & Methods in Physics Research. Section B: Beam Interactions with Materials and Atoms. 449, p. 17-21 5 p.

### **Analytical interatomic bond-order potential for simulations of oxygen defects in iron**

Byggmästar, J. J. A., Nagel, M. J., Albe, K., Henriksson, K. O. E. & Nordlund, K. H., 29 May 2019, In : Journal of Physics. Condensed Matter. 31, 21, 11 p., 215401.

### **Velocity-dependent dark matter interactions in single-electron resolution semiconductor detectors with directional sensitivity**

Heikinheimo, M., Nordlund, K., Tuominen, K. & Mirabolfathi, N., 29 May 2019, In : Physical Review D. 99, 10, 11 p., 103018.

### **Molecular dynamics simulation of beryllium oxide irradiated by deuterium ions: sputtering and reflection**

Hodille, E. A., Byggmästar, J., Safi, E. & Nordlund, K., 8 May 2019, In : Journal of Physics. Condensed Matter. 31, 18, 17 p., 185001.

### **Site-Specific Wetting of Iron Nanocubes by Gold Atoms in Gas-Phase Synthesis**

Vernieres, J., Steinhauer, S., Zhao, J., Grammatikopoulos, P., Ferrando, R., Nordlund, K., Djurabekova, F. & Sowwan, M., 2 May 2019, In : Advanced Science. 6, 13, 8 p., 1900447.

### **Gas-Phase Synthesis of Trimetallic Nanoparticles**

Mattei, J-G., Grammatikopoulos, P., Zhao, J., Singh, V., Vernieres, J., Steinhauer, S., Porkovich, A., Danielson, E., Nordlund, K., Djurabekova, F. & Sowwan, M., 26 Mar 2019, In : Chemistry of Materials. 31, 6, p. 2151-2163 13 p.

### **Radiation stability of nanocrystalline single-phase multicomponent alloys**

Levo, E., Granberg, F., Utt, D., Albe, K., Nordlund, K. & Djurabekova, F., 14 Mar 2019, In : Journal of Materials Research. 34, 5, p. 854-866 13 p.

### **Modeling of high-fluence irradiation of amorphous Si and crystalline Al by linearly focused Ar ions**

Lopez-Cazalilla, A., Ilinov, A., Nordlund, K. & Djurabekova, F., 20 Feb 2019, In : Journal of Physics. Condensed Matter. 31, 7, 13 p., 075302.

### **A locked mode indicator for disruption prediction on JET and ASDEX upgrade**

Sias, G., Cannas, B., Fanni, A., Murari, A., Pau, A., ASDEX Upgrade Team, EUROfusion MST1 Team, JET Contributors, Aho-Mantila, L., Costea, S., Holm, J. H., Zhang, W., Dimitrova, M., Lahtinen, A., Marchand, B., Ahlgren, T., Bjorkas, C., Heinola, K., Järvinen, A., Makkonen, T. & 2 othersNordlund, K. & Safi, E., Jan 2019, In : Fusion Engineering and Design. 138, p. 254-266 13 p.

### **Modelling of radiation damage in materials**

Nordlund, K. H. & Short, M., 2019, *Handbook of materials modelling: Methods: Theory and Modeling*. Andreoni, W. & Yip, S. (eds.). 2nd ed. Cham: Springer International Publishing AG

### **Molecular dynamics simulations of non-equilibrium systems**

Nordlund, K. H. & Djurabekova, F. G., 2019, *Handbook of materials modelling: Methods: Theory and Modeling*. Andreoni, W. & Yip, S. (eds.). 2nd ed. Cham: Springer International Publishing AG

### **Radiation damage in tungsten from cascade overlap with voids and vacancy clusters**

Fellman, A. J. J., Sand, A., Byggmästar, J. & Nordlund, K., 2019, In : Journal of Physics. Condensed Matter. 31, 40, 12 p., 405402.

### **Primary radiation damage: A review of current understanding and models**

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### **The Compact Linear e<sup>+</sup>e<sup>-</sup> Collider (CLIC): 2018 Summary Report**

CLIC Collaboration, CLICdp Collaboration, Charles, T. K., Aicheler, M., Baibuz, E., Brücken, E., Djurabekova, F., Eerola, P., Garcia, F., Haeggström, E., Huitu, K., Jansson, V., Kassamakov, I., Kimari, J., Kyrtsakis, A., Lehti, S., Meriläinen, A., Montonen, R., Nordlund, K., Österberg, K. & 5 othersSaessalo, A., Väinölä, J., Veske, M., Vigonski, S. & Zadin, V., 14 Dec 2018, Geneva: CERN. 112 p. (CERN Yellow Reports: Monographs ; vol. 2/2018, no. CERN-2018-005-M)

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### **Defect structures and statistics in overlapping cascade damage in fusion-relevant bcc metals**

Sand, A. E., Byggmästar, J., Zitting, A. & Nordlund, K., 1 Dec 2018, In : Journal of Nuclear Materials. 511, p. 64-74 11 p.

### **Defect Creation in Crystals: A Portal to Directional Dark Matter Searches**

Kadribasic, F., Mirabolfathi, N., Nordlund, K., Holmström, E. & Djurabekova, F., Dec 2018, In : Journal of Low Temperature Physics. 193, 5-6, p. 1146-1150 5 p.

### **Effect of random surface orientation on W sputtering yields**

Jussila, J., Granberg, F. & Nordlund, K., Dec 2018, In : Nuclear Materials and Energy. 17, p. 113-122 10 p.

### **Dependence of ion channeling on relative atomic number in compounds**

Nordlund, K. & Hobler, G., 15 Nov 2018, In : Nuclear Instruments & Methods in Physics Research. Section B: Beam Interactions with Materials and Atoms. 435, p. 61-69 9 p.

### **Varje dag kolliderar vi med exotiska rymdpartiklar**

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### **A model of defect cluster creation in fragmented cascades in metals based on morphological analysis**

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### **Vaporlike phase of amorphous SiO<sub>2</sub> is not a prerequisite for the core/shell ion tracks or ion shaping**

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### **Effects of the short-range repulsive potential on cascade damage in iron**

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### **Molecular Dynamics Simulations of Heavy Ion Induced Defects in SiC Schottky Diodes**

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### **Analytical bond order potential for simulations of BeO 1D and 2D nanostructures and plasma-surface interactions**

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### **Directional Sensitivity in Light-Mass Dark Matter Searches with Single-Electron-Resolution Ionization Detectors**

Kadribasic, F., Mirabolfathi, N., Nordlund, K., Sand, A. E., Holmström, E. & Djurabekova, F., 16 Mar 2018, In : Physical Review Letters. 120, 11, 5 p., 111301.

### **Improving atomic displacement and replacement calculations with physically realistic damage models**

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### **Nanohajpen: finns tekniken ingenstans eller överallt?**

Nordlund, K. H., 5 Mar 2018, In : Forum för ekonomi och teknik. 2

### **Graphitization of amorphous carbon by swift heavy ion impacts: Molecular dynamics simulation**

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#### **Slowing down of 100keV antiprotons in Al foils**

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#### **Analysis of Defect Formation in High-Fluence Ion Mixing in Si-SiO<sub>2</sub> Nanolayers**

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#### **Effects of crystallographic and geometric orientation on ion beam sputtering of gold nanorods**

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#### **Absence of single critical dose for the amorphization of quartz under ion irradiation**

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#### **Simulation of redistributive and erosive effects in a-Si under Ar<sup>+</sup> irradiation**

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#### **Formation and emission mechanisms of Ag nanoclusters in the Ar matrix assembly cluster source**

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#### **Molecular dynamics simulations of thermally activated edge dislocation unpinning from voids in $\alpha$ -Fe**

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#### **MD and SCA simulations of He and H bombardment of fuzzi in bcc elements**

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#### **Simulation of Ion Beam Mixing in Si/SiO<sub>2</sub>/Si Pillars with Accelerated Molecular Dynamics**

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**Thermal Oxidation of Size-Selected Pd Nanoparticles Supported on CuO Nanowires: The Role of the CuO–Pd Interface**  
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**Multi-Scale Modelling to Relate Beryllium Surface Temperature, Deuterium Concentration and Erosion in Fusion Reactor Environment**  
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**Gas Phase Synthesis of Multifunctional Fe-Based Nanocubes**  
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**Formation of Meta-Stable SiO<sub>x</sub> by Ion Beam Mixing for Self-Assembly of a Si Nanodot**  
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**Damage buildup and edge dislocation mobility in equiatomic multicomponent alloys**  
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**CASCADE DEBRIS OVERLAP MECHANISM OF <100> DISLOCATION LOOP FORMATION IN Fe AND FeCr**  
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#### **Creating nanoporous graphene with swift heavy ions**

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#### **A LOW-LEVEL DETECTION SYSTEM FOR HYDROGEN ANALYSIS WITH THE REACTION $1\text{H}(15\text{N},\alpha\text{-GAMMA})12\text{C}$**

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## **Projects**

### **Materials- and Nanophysics Researcher Community (MATENA)**

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22/02/2011 → ...

#### **Nanohiukkasten optiset ja pintaominaisuudet**

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Suomen Akatemia  
01/01/2007 → 31/12/2010

#### **MachQu: Probabilistic Machine Learning for Quantum Mechanics-Based Material Design**

Roos, T., Djurabekova, F. & Nordlund, K.  
01/01/2018 → 31/12/2019

## **Activities**

### **Insights on sputtering and deposition mechanisms from molecular dynamics simulations**

Kai Nordlund (Speaker)  
7 Dec 2018

### **Possibility of materials modification by dark matter particle irradiation**

Kai Nordlund (Speaker)  
27 Nov 2018

### **Improving on analytical radiation damage calculations: arc-dpa and rpa**

Kai Nordlund (Speaker)  
16 Oct 2018

### **Fundamental mechanisms of accelerated and plasma ion interactions with materials: insights from atomistic simulations**

Kai Nordlund (Speaker)  
21 Jun 2018

### **Channeling effects in nanostructures: analysis and comparisons with experiments**

Kai Nordlund (Speaker)  
13 Apr 2018

### **Nuclear stopping power of antiprotons**

Kai Nordlund (Speaker)  
14 Mar 2018

### **Molecular dynamics simulations of collision cascades: method developments and results from 1993 on**

Kai Nordlund (Speaker)  
7 Dec 2017

### **High-dose damage evolution in Fe, FeCr, and high-entropy alloys**

Kai Nordlund (Speaker)  
15 Nov 2017

### **Improving atomic displacement calculations with physically realistic damage models: arc-dpa and rpa**

Kai Nordlund (Speaker)  
25 Oct 2017

**Systematic analysis of ion channeling over all crystal directions: dependences on energy, crystal structure, atom size, temperature, and defect concentration**

Kai Nordlund (Speaker)  
24 Oct 2017

**Insights to physics of sputtering and channeling effects learnt from molecular dynamic simulations**

Kai Nordlund (Speaker)  
21 Aug 2017

**Current topics of modelling in materials science (in Helsinki)**

Kai Nordlund (Speaker), Flyura Gatifovna Djurabekova (Speaker)  
3 Aug 2017

**20th INTERNATIONAL CONFERENCE ON SURFACE MODIFICATION OF MATERIALS BY ION BEAMS**

Kai Nordlund (Attendee)  
11 Jul 2017

**Nanoscale pattern formation at surfaces and Formation of 3D nanostructures**

Flyura Djurabekova (Chair), Kai Henrik Nordlund (Chair), Christoffer John Patrik Fridlund (Member of organizing committee), Andrew Ilinov (Secretary of organizing committee), Alvaro Lopez Cazalilla (Member of organizing committee), Antti Armas Kuronen (Scientific Committee Vice Chair)  
26 Jun 2017 → 30 Jun 2017

**Tutorial: atomistic simulations for irradiation effects.**

Kai Nordlund (Speaker)  
15 Nov 2016

**International conference on metallurgical coatings and thin films (ICMCTF)**

Kai Nordlund (Speaker: Keynote)  
2016

**MRS fall meeting, symposium Ion Beam Enabled Nanoscale Fabrication and Materials Synthesis**

Kai Nordlund (Speaker: Keynote)  
2016

**Summer school on plasma-surface interactions**

Kai Nordlund (Speaker: Presenter)  
2016

**Workshop on nanocluster deposition**

Kai Nordlund (Speaker: Keynote)  
2016

**Fysiikan päivät 2015**

Kai Nordlund (Speaker: Keynote)  
17 Mar 2015

**CECAM workshop on Modeling metal-based nanoparticles: toward realistic environments**

Kai Nordlund (Speaker: Keynote)  
2015

**International Symposium on Multi-scale Modeling and Simulation of Materials**

Kai Nordlund (Speaker: Keynote)  
2015

**MRS Fall Meeting, symposium Defect and Radiation Effects in Advanced Materials**

Kai Nordlund (Speaker: Keynote)

2015

**MRS Spring Meeting, symposium Multiscale modeling of microstructural evolution in nuclear materials**

Kai Nordlund (Speaker: Keynote)

2015

**Radiation Effects in Insulators School, Invited tutorial talk**

Kai Nordlund (Speaker: Keynote)

2015

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)

2015

**Director of MATRENA doctoral programme**

Kai Nordlund (Director)

1 Jan 2014 → ...

**18th International Conference on Surface Modification of Materials by Ion Beams**

Kai Nordlund (Speaker: Keynote)

2014

**2014 Nuclear materials Conference**

Kai Nordlund (Speaker: Keynote)

2014

**22nd International Conference on Ion-Surface Interactions**

Kai Nordlund (Speaker: Keynote)

2014

**EMRS Spring meeting, Symposium Defect-induced effects in nanomaterials**

Kai Nordlund (Speaker: Keynote)

2014

**EUROFusion (External organisation)**

Kai Nordlund (Member)

2014 → ...

**European Grid Infrastructure Community Forum**

Kai Nordlund (Chair)

2014

**International Atomic Energy Agency (External organisation)**

Kai Nordlund (Expert member)

2014 → 2017

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)

2014

**Radiation Effects in Insulators**

Kai Nordlund (Chair)  
30 Jun 2013 → 5 Jul 2013

**8th symposium of the International Society for Theoretical Chemical Physics**

Kai Nordlund (Speaker: Keynote)  
2013

**EMRS Spring meeting, Symposium Ion Beam Applications: New and Innovative Approaches**

Kai Nordlund (Speaker: Keynote)  
2013

**IUMRS-ICAM Modeling & Simulation Session**

Kai Nordlund (Chair)  
2013

**International Atomic Energy Agency (External organisation)**

Kai Nordlund (Expert member)  
2013 → 2017

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)  
2013

**3rd EU-Russia Innovation Forum**

Kai Nordlund (Speaker: Keynote)  
2012

**All-Russian Conference in Physical and physico-chemical bases of ion implantation**

Kai Nordlund (Speaker: Keynote)  
2012

**Harriet Åhlgren, PhD thesis co-supervision**

Kai Nordlund (Co-supervisor)  
2012 → 2015

**International supercomputing conference**

Kai Nordlund (Speaker: Keynote)  
2012

**Joint ICTP-IAEA workshop on Fusion Plasma Modelling**

Kai Nordlund (Speaker: Keynote)  
2012

**Recent developments in the study of radiation effects in matter (REM) invitation-only meeting**

Kai Nordlund (Speaker: Presenter)  
2012

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)  
2012

**international committee for conference series Ion Beam Modification of Materials (IBMM) (External organisation)**

Kai Nordlund (Board member)  
2012 → ...

**International Committee for Radiation Effects in Insulators (REI) conference (External organisation)**

Kai Nordlund (Board member)

2011 → 2015

**20th International Conference on Ion-Surface Interactions**

Kai Nordlund (Attendee)

2011

**Aleksi A Leino, PhD thesis co-supervision**

Kai Nordlund (Co-supervisor)

2011 → 2015

**Andrea Sand, PhD thesis supervision**

Kai Nordlund (Supervisor)

2011 → 2015

**Andrey Ilinov, PhD thesis co-supervision**

Kai Nordlund (Co-supervisor)

2011 → 2015

**Breakdown Physics Workshop (MeVArc)**

Kai Nordlund (Chair)

2011

**EMRS/IUMRS/ICAM Spring meeting 2011 symposium 'Ion and cluster ion beams for the synthesis and controlled modification of nanomaterials'**

Kai Nordlund (Chair)

2011

**Fall MRS 2011 meeting, symposium Self-organization and nanoscale pattern formation**

Kai Nordlund (Speaker: Keynote)

2011

**Konstantin Avchachiov, PhD thesis supervision**

Kai Nordlund (Co-supervisor)

2011 → 2015

**OECD Nuclear Energy Agency (External organisation)**

Kai Nordlund (Chair)

2011 → 2015

**PRACE Summer School for advanced programming of Tier-0 supercomputers**

Kai Nordlund (Speaker: Keynote)

2011

**Spring MRS meeting, symposium Ion Beams – New Applications from the Mesoscale to Nanoscale**

Kai Nordlund (Speaker: Keynote)

2011

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)

2011



**18th International Workshop on Inelastic Ion-Surface Collisions**

Kai Nordlund (Speaker: Keynote)  
2010

**24th International Conference on Atomic Collisions in Solids**

Kai Nordlund (Speaker: Keynote)  
2010

**CECAM workshop on radiation damage and non-adiabatic simulations**

Kai Nordlund (Speaker: Keynote)  
2010

**CIMTEC 2010 - 12th International Ceramics Congress & 5th Forum on New Materials**

Kai Nordlund (Speaker: Keynote)  
2010

**Mohammad Wali Ullah, PhD thesis supervision**

Kai Nordlund (Co-supervisor)  
2010 → 2014

**OECD Nuclear Energy Agency (External organisation)**

Kai Nordlund (Chair)  
2010 → 2014

**SPIE Photonics West Meeting on Synthesis and Photonics of Nanoscale Materials VII (SPnsM-VII)**

Kai Nordlund (Speaker: Keynote)  
2010

**Spring MRS meeting, symposium Materials for Nuclear Applications and Extreme Environments**

Kai Nordlund (Speaker: Keynote)  
2010

**Towards Reality in Nanoscale Materials**

Kai Nordlund (Chair)  
2010

**Aarne Pohjonen, PhD thesis co-supervision**

Kai Nordlund (Co-supervisor)  
2009 → 2013

**Ane Lasa, PhD thesis supervision**

Kai Nordlund (Supervisor)  
2009 → 2013

**Eero Holmström, PhD thesis supervision**

Kai Nordlund (Supervisor)  
2009 → 2012

**Helga Timko, PhD thesis supervision**

Kai Nordlund (Co-supervisor)  
2009 → 2011

**Nanostructures in silica**

Kai Nordlund (Chair)  
2009

**Ville Jansson, PhD thesis co-supervision**

Kai Nordlund (Co-supervisor)  
2009 → 2013

**Ville Jansson, PhD thesis supervision**

Kai Nordlund (Co-supervisor)  
2009 → 2013

**Katharina Vörtler, PhD thesis supervision**

Kai Nordlund (Supervisor)  
2008 → 2011

**Marie Backman, PhD thesis supervision**

Kai Nordlund (Co-supervisor)  
2008 → 2012

**Antti Tolvanen, Co-Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2007 → 2010

**Jussi Polvi, PhD thesis supervision**

Kai Nordlund (Supervisor)  
2007 → 2013

**Ari Harjunmaa, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2006 → 2011

**Carolina Björkas, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2006 → 2009

**Niklas Juslin, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2006 → 2009

**Tommi Järvi, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2006 → 2009

**Invited talks at international conferences 2005 - 2010**

Kai Nordlund (Speaker: Presenter)  
1 Jan 2005 → 31 Dec 2010

**Co-supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2005 → 2007

**Juha Samela, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2005 → 2008

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2004 → 2009

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2002 → 2006

**Krister Henriksson, Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2001 → 2005

**International Committee for the Computer simulation of radiation effects in solids (COSIRES) conference (External organisation)**

Kai Nordlund (Board member)  
2000 → ...

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2000 → 2003

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2000 → 2003

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
2000 → 2004

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
1999 → 2002

**Supervision of PhD student**

Kai Nordlund (Supervisor)  
1997 → 2000

**Supervision of PhD thesis**

Kai Nordlund (Supervisor)  
1997 → 2000

**Yunzheng Zhong, Co-supervision of PhD thesis**

Kai Nordlund (Co-supervisor)  
1997 → 1999