

Thuat T. Trinh

Curriculum Vitæ (March 8, 2017)

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EXPERIENCES

Visiting researcher 2017-present
Center for Innovative Materials and Architectures, INOMAR, HoChiMinh City, Vietnam

Visiting researcher 2016-present
Ton Duc Thang University, HoChiMinh City, Vietnam

Senior Engineer 2017-present
Dept. of Civil and Environmental Engineering, NTNU, Norway

Researcher 2011-2016
Dept. of Chemistry, NTNU, Norway

Postdoctoral Fellow 2009-2011
Ecole Normale Supérieure de Lyon, France

EDUCATION

PhD in Chemistry and Chemical Engineering 2004-2009
Eindhoven University of Sci. and Tech., The Netherlands

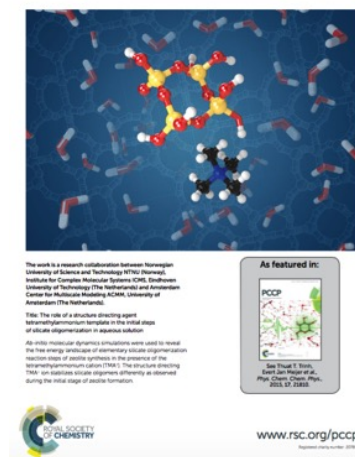
M.Sc. Material Science 2003-2004
Institute Polytechnique de Toulouse-ENSIACET, France

B.Sc Chemistry 1999-2003
Dept. of Chemistry, University of Science, Vietnam National University of HoChiMinh city, Vietnam

RESEARCH AND PUBLICATIONS

Over 35 published works in professional, high-impact journals including Phys.Chem.Chem. Phys, Nature. Communications., Physical Review Letters, Angewandte Chemie, J. Am. Chem. Soc)

Journal Cover: Back cover of Phys. Chem. Chem. Phys, 2015, issue 34



Pulication list

40. **Thuat T. Trinh**, Nora Melding, Dick Bedeaux and Signe Kjelstrup, [Thermodynamic Properties of Hydrogen Dissociation Reaction from the Small System Method and Reactive Force Field ReaxFF](#), *Chem. Phys. Lett* 2017, 672,128
39. Eirik Hjertenæs, **Thuat T. Trinh**, and Henrik Koch, [Chemically accurate energy barriers of small gas molecules in through hexagonal water ringst](#), *Phys. Chem. Chem. Phys*, 2016, 18, 17831
38. **Thuat T. Trinh**, Xavier Rozanska, Françoise Delbecq, Alain Tuel and Philippe Sautet, [The mechanism of the initial step of germanosilicate formation in solution: a first-principles molecular dynamics study](#), *Phys. Chem. Chem. Phys*, 2016, 18, 14419
37. R. Rurali, L. Colombo, X. Cartoixa, Ø. Wilhelmsen, **T. T. Trinh**, D. Bedeaux, and S. Kjelstrup, [Heat transportthrough a solid-solid junction: the interface as an autonomous thermodynamicsystem](#), *Phys. Chem. Chem. Phys*, 2016, 18, 13741
36. Øivind Wilhelmsen, **Thuat T. Trinh**, Anders Lervik, Vijay Kumar Badam, Signe Kjelstrup, and Dick Bedeaux, [Coherent description of transport across the water interface: From nanodroplets to climate models](#), *Phys. Rev. E*, 2016, 93, 32801
35. Anders Lervik, Øivind Wilhelmsen, **Thuat Trinh**, and Edgar Blokhuis, ["A new truncation correction for the configurational temperature extends its applicability to interaction potentials with a discontinuous force"](#), *J. Chem. Phys*, 2016, accepted
34. **Thuat T. Trinh**, Khanh-Quang Tran, Quang-Vu Bach, Dao Q. Trinh, ["A Molecular Dynamics Simulation Study on Separation Selectivity of CO₂/CH₄ Mixture in Mesoporous Carbons"](#), *Energy Procedia*, 2016, 86, 144

33. Mahmoud Moqadam, Enrico Riccardi, **Thuat Trinh**, Per-Olof Astrand, and Titus van Erp, "A test on reactive forcefields for the study of silica dimerization reactions", *J. Chem. Phys.*, 2015, 143, 184113
32. Jianyang Wu, Fulong Ning, **Thuat Trinh**, Signe Kjelstrup, Thijs J. H. Vlugt, Jianying He, Bjørn H. Skallerud, and Zhiliang Zhang, "Mechanical Instability of Monocrystalline and Polycrystalline Methane Hydrates", *Nature Communications*, 2015, 6, 8743
31. Mehandzhiyski, Aleksandar; Riccardi, Enrico; van Erp, Titus; Koch, Henrik; Åstrand, Per-Olof; **Trinh, Thuat**; Grimes, Brian, "DFT Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids", *J. Phys. Chem. A*, 2015, 119 (40), 10195-10203
30. Anders Lervik, Øivind Wilhelmsen, **Thuat Trinh**, and Henrik R. Nagel, "Finite-size and truncation effects for microscopic expressions for the temperature at equilibrium and nonequilibrium", *J. Chem. Phys.* 143, 114106 (2015)
29. Mehandzhiyski, Aleksandar; Riccardi, Enrico; van Erp, Titus; **Trinh, Thuat**; Grimes, Brian, "Ab-initio Molecular Dynamics Study on the Interactions between Carboxylate Ions and Metal Ions in Water", *J. Phys. Chem. B*, 2015, 119 (33), pp 10710–10719
28. **Thuat T Trinh**, Khanh-Quang Tran, Xue-Qing Zhang, Rutger A van Santen and Evert Jan Meijer, "The role of a structure directing agent tetramethylammonium template in the initial step of silicate oligomerization in aqueous solution", *Phys. Chem. Chem. Phys.*, 2015, 17, 21810-21818
27. Victorio Saez Talens, Pablo Englebienne, **Thuat T. Trinh**, Willem E. M. Noteborn, Ilja K. Voets, Roxanne E. Kieltyka, "Aromatic gain in a supramolecular polymer, *Angewandte Chemie*, 2015, <http://onlinelibrary.wiley.com/doi/10.1002/anie.201503905/full>
26. Bach, Quang Vu; Tran, Khanh-Quang; Skreiberg, Øyvind; **Trinh, Thuat**. "Effects of Wet Torrefaction on Pyrolysis of Woody Biomass Fuels" *Energy*, 2015, 88, 443
25. **Thuat T. Trinh**, Magnus H. Waage, Titus S. van Erp, and Signe Kjelstrup, "Communication "Low barriers for hydrogen diffusion in sII clathrate", *Phys. Chem. Chem. Phys.*, 2015, 17, 13808-13812
24. Mazzola, Federico; **Trinh, Thuat**; Cooil, Simon; Østli, Elise; Hoydalsvik, Kristin; Skjønsvjell Bakken, Eirik; Kjelstrup, Signe; Preobrajenski, Alexei; Cafolla, Tony; Evans, Andrew; Breiby, Dag; Wells, Justin, "Graphene coatings for chemotherapy; Avoiding silver-mediated degradation", *IOP:2D Material*, invited, [doi:10.1088/2053-1583/2/2/025004](https://doi.org/10.1088/2053-1583/2/2/025004)
23. Wilhelmsen, Øivind; **Trinh, Thuat**; Kjelstrup, Signe; Bedeaux, Dick. "The Influence of Curvature on the Transfer Coefficients for Evaporation and Condensation of the Lennard-Jones Fluid from Square-Gradient Theory and Nonequilibrium Molecular Dynamics." *Journal of Physical Chemistry C* 2015, 119, 8160–8173
22. **Thuat T Trinh**, Signe Kjelstrup, Dick Bedeaux, Titus van Erp and Carlos Grande, "A procedure to find thermodynamic equilibrium constants for co2 and ch4 adsorption on activated carbon" *Phys. Chem. Chem. Phys.*, 2015, 17, 8223
21. **Trinh, Thuat**; Vlugt, Thijs J.H.; Hagg, May-Britt; Bedeaux, Dick; Kjelstrup, Signe "Simulation of Pore Width and Pore Charge Effects on Selectivities of CO2 vs. H2 from a Syngas-like Mixture in Carbon Mesopores", *Energy Procedia* 2015, 64, 150-159

20. Øivind Wilhelmsen, **Thuat Trinh**, Signe Kjelstrup, Dick Beadeaux, Titus v. Erp. "Heat and mass transfer across interfaces in complex nanogeometries", *Physical Review Letters*, 2015, 114, 065901.
19. **T.T. Trinh**, D. Bedeaux, J.-M Simon and S. Kjelstrup, "Calculation of chemical potential and activity coefficient of two layers of CO₂ adsorbed on a graphite surface", *Phys. Chem. Chem. Phys* (2015), 17, 1226. DOI: 10.1039/c4cp03782k
18. **Trinh, Thuat**; Vlugt, Thijs J.H.; Kjelstrup, Signe. Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics: a systematic study of several common force fields. *Journal of Chemical Physics* 2014, 141, 134504
17. Tran, Khanh-Quang; Bach, Quang Vu; **Trinh, Thuat**; Seisenbaeva, Gulaim. "Non-isothermal pyrolysis of torrefied stump - A comparative kinetic evaluation". *Applied Energy*, (2014), 216,759
16. Kjelstrup S, Schnell SK, Vlugt TJ, Simon J-M, Bardow A, Bedeaux D, **Trinh TT**. Bridging scales with thermodynamics: from nano to macro. *Advances in Natural Sciences: Nanoscience and Nanotechnology*. 2014;5(2):023002.
15. van Erp TS, **Trinh TT**, Kjelstrup S, Glavatskiy K. On the relation between the Langmuir and thermodynamic flux equations. *Frontier of Physics*. 2014;1:36.
14. **Trinh T**, Bedeaux D, Simon J-M, Kjelstrup S. Thermodynamic Characterization Of Two Layers Of CO₂ On A Graphite Surface. *Chemical Physics Letters*. 2014, 612, 214
13. Pavlova A, **Trinh TT**, van Santen RA, Meijer EJ. Clarifying the role of sodium in the silica oligomerization reaction. *Physical Chemistry Chemical Physics*. 2013;15(4):1123-9.
12. **Trinh T**, Vlugt T, Hägg M, Bedeaux D, Kjelstrup S, editors. Simulating CO₂ adsorption and diffusion on a graphite SURFACE. 12th Joint European Thermodynamics Conference; 2013.
11. **Trinh TT**, Vlugt TJ, Hägg M-B, Bedeaux D, Kjelstrup S. Selectivity and self-diffusion of CO₂ and H₂ in a mixture on a graphite surface. *Frontiers in chemistry*. 2013;1.
10. **Trinh TT**, Rozanska X, Delbecq F, Sautet P. The initial step of silicate versus aluminosilicate formation in zeolite synthesis: a reaction mechanism in water with a tetrapropylammonium template. *Physical Chemistry Chemical Physics*. 2012;14(10):3369-80.
9. Zhang X-Q, **Trinh TT**, van Santen RA, Jansen AP. Mechanism of the initial stage of silicate oligomerization. *Journal of the American Chemical Society*. 2011;133(17):6613-25.
8. Zhang X-Q, **Trinh TT**, van Santen RA, Jansen AP. Structure-directing role of counterions in the initial stage of zeolite synthesis. *The Journal of Physical Chemistry C*. 2011;115(19):9561-7.
7. Szyja B, Vassilev P, **Trinh T**, van Santen R, Hensen E. The relative stability of zeolite precursor tetraalkylammonium-silicate oligomer complexes. *Microporous and Mesoporous Materials*. 2011;146(1):82-7.
6. Zhang X-Q, **Trinh TT**, van Santen RA, Jansen AP. Reply to "Comment on 'Structure-Directing Role of Counterions in the Initial Stage of Zeolite Synthesis'". *The Journal of Physical Chemistry C*. 2011;116(1):1622-3.

5. **Trinh TT**, Jansen AP, van Santen RA, Meijer EJ. [Role of water in silica oligomerization](#). The Journal of Physical Chemistry C. 2009;113(7):2647-52.
4. **Trinh TT**, Jansen AP, van Santen RA, Meijer EJ. [The role of water in silicate oligomerization reaction](#). Physical Chemistry Chemical Physics. 2009;11(25):5092-9. (Hot PCCP article)
3. **Trinh TT**, Jansen AP, van Santen RA, VandeVondele J, Meijer EJ. [Effect of counter ions on the silica oligomerization reaction](#). ChemPhysChem. 2009;10(11):1775-82.
2. **Thuat T. Trinh**. [A computational study of silicate oligomerization reactions](#): PhD thesis, Eindhoven University of Technology; 2009.
1. **Trinh TT**, Jansen AP, van Santen RA. [Mechanism of oligomerization reactions of silica](#). The Journal of Physical Chemistry B. 2006;110(46):23099-106.

SYNERGISTIC ACTIVITIES

- Associate Editor: Frontiers in Chemistry, Frontiers in Physics
- Referee for journal: Phys. Chem. Chem. Phys ; J. Phys. Chem. B.; J. Chem. Phys.; Compt. Mat. Sci., Scientific Report, ...
- Active member of: Norsk Kjemisk Selskap, Assian Consortium on Computational Materials Science.