

List of publications: Dr. Ragnar Björnsson

2021

- Cipriani, M., **Björnsson, R.**, Barclay, M., Terfort, A., Fairbrother, H., Ingólfsson, O. (2020). Relative cross sections and appearance energies in electron impact ionization and dissociation of mono-halogenated biphenyls *International Journal of Mass Spectrometry* 459, 116452. <https://doi.org/10.1016/j.ijms.2020.116452>

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- Ghosh, D., **Björnsson, R.**, Damodaran, K.K. (2020). Role of N–Oxide Moieties in Tuning Supramolecular Gel-State Properties *Gels* 6(4), 41. <https://doi.org/10.3390/gels6040041>
- Martin, H., Somers, T., Dwyer, M., Robson, R., Pfeffer, F.M., **Björnsson, R.**, Krämer, T., Kavanagh, K., Velasco-Torrijos, T. (2020). Scaffold Diversity for Enhanced Activity of Glycosylated Inhibitors of Fungal Adhesion *RSC Medicinal Chemistry* 11(12), 1386-1401. <https://doi.org/10.1039/D0MD00224K>
- Benediktsson, B., **Björnsson, R.** (2020). Quantum Mechanics/Molecular Mechanics Study of Resting-State Vanadium Nitrogenase: Molecular and Electronic Structure of the Iron–Vanadium Cofactor *Inorganic Chemistry* 59(16), 11514-11527. <https://doi.org/10.1021/acs.inorgchem.0c01320>
- Rodríguez-Maciá, P., Galle, L., **Björnsson, R.**, Lorent, C., Zebger, I., Yoda, Y., Cramer, S., DeBeer, S., Span, I., Birrell, J.A. (2020). Caught in the H_{inact}: Crystal Structure and Spectroscopy Reveal a Sulfur Bound to the Active Site of an O₂-stable State of [FeFe] Hydrogenase *Angewandte Chemie International Edition* 59(38), 16786-16794. <https://doi.org/10.1002/anie.202005208>
- Van Stappen, C., Decamps, L., Cutsail III, G.E., **Björnsson, R.**, Henthorn, J.T., Birrell, J.A., DeBeer, S. (2020). The Spectroscopy of Nitrogenases *Chemical Reviews* 120(12), 5005-5081. <https://doi.org/10.1021/acs.chemrev.9b00650>
- Thorarinsdottir, A.E, Björnsson, R., Harris, T.D. (2020). Insensitivity of Magnetic Coupling to Ligand Substitution in a Series of Tetraoxolene Radical-Bridged Fe₂ Complexes *Inorganic Chemistry* 59(7), 4634-4649. <https://doi.org/10.1021/acs.inorgchem.9b03736>
- Da Silva, F.F., Thorman, R.M., **Björnsson, R.**, Lu, H., McElwee-White, L., Ingólfsson, O. (2020). Dissociation of the FEBID precursor *cis*-Pt(CO)₂Cl₂ driven by low-energy electrons *Physical Chemistry Chemical Physics* 22(11), 6100-6108. <https://doi.org/10.1039/C9CP06633K>

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- Thorhallsson, A.Th., Benediktsson, B., **Björnsson, R.** (2019). A model for dinitrogen binding in the E₄ state of nitrogenase *Chemical Science* 10(48), 11110-11124. <https://doi.org/10.1039/c9sc03610e>
- Van Stappen, C., Thorhallsson, A.T., Decamps, L., **Björnsson, R.**, DeBeer, S. (2019). Resolving the structure of the E₁ state of Mo Nitrogenase through Mo and Fe K-edge EXAFS and QM/MM calculations *Chemical Science* 10(42), 9807-9821. <https://doi.org/10.1039/c9sc02187f>

- Barclay, M., **Bjornsson, R.**, Cipriani, M., Terfort, A., Fairbrother, D.H., Ingólfsson, O. (2019). The role of the dihedral angle and excited cation states in ionization and dissociation of mono-halogenated biphenyls; a combined experimental and theoretical coupled cluster study *Physical Chemistry Chemical Physics* 21, 4556-4567. <https://doi.org/10.1039/c8cp07785a>
- Thorhallsson, A.Th., **Bjornsson, R.** (2019). Computational Mechanistic Study of [MoFe₃S₄] Cubanes for Catalytic Reduction of Nitrogenase Substrates *Inorganic Chemistry* 58(3), 1886-1894. <https://doi.org/10.1021/acs.inorgchem.8b02669>
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- Benediktsson, B., Thorhallsson, A.T., **Bjornsson, R.** (2018). QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure *Chemical Communications* 54, 7310-7313. <https://doi.org/10.1039/C8CC03793K>
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- Abbehausen, C., Ferraz de Paiva, R.E., **Bjornsson, R.**, Quintana Gomes, S., Du, Z., Corbi, P.P., Lima, F.A., Farrell, N. (2018) X-ray Absorption Spectroscopy Combined with Time-Dependent Density Functional Theory Elucidates Differential Substitution Pathways of Au(I) and Au(III) with Zinc Fingers *Inorganic Chemistry* 57(1), 218-230. <https://doi.org/10.1021/acs.inorgchem.7b02406>

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- T P., R.K., **Bjornsson, R.**, Barth, S., Ingólfsson, O. (2017). Formation and decay of negative ion states up to 11 eV above the ionization energy of the nanofabrication precursor HFeCo₃(CO)₁₂ *Chemical Science* 8(9), 5949-5952. <https://doi.org/10.1039/c7sc01927k>
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- Sigurdardóttir, B.K., Kvaran, A., **Bjornsson, R.**, Arnason, I. (2016). Dissociative Photoionization of 1-Halogenated Silacyclohexanes: Silicon Traps the Halogen *The Journal of Physical Chemistry A* 120(46), 9188-9197. <https://doi.org/10.1021/acs.jpca.6b09195>
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- **Bjornsson, R.**, Neese, F., Schrock, R.R., Einsle, O., DeBeer, S. (2015). The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry *Journal of Biological Inorganic Chemistry* 20(2), 447-460. <https://doi.org/10.1007/s00775-014-1230-6>
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