Tentative Outline

Title of the Thematic Issue: Discovering High-Performance Electro-Chemical Catalysts for Nitrogen Reduction Through Computational Approaches

Guest Editor: Dr. Huilong Dong

Aims & Scope:

Ammonia (NH_3) is the most highly produced compounds in the chemical industry. Considering the tremendous energy costed by traditional Haber-Bosch process, nitrogen reduction reaction (NRR) catalyzed by electro-chemical approach has received great scientific attentions. Despites the experimental efforts, computational simulations have been another efficient way to find out stable and high-performance electro-chemical catalysts for NRR. In this Special Issue, we would like to provide a platform for theoretical researchers to share their recent findings on discovering the novel NRR electro-catalysts.

All researchers working in the field are cordially invited to contribute with original research papers or reviews to this Special Issue, reporting on screening & design of novel materials as NRR electro-catalysts, mechanism explanation of NRR, or theoretical aided experimental findings of NRR process.

Keywords: Electro-catalyst, Nitrogen reduction reaction, Computational simulations, NH_3.

Subtopics: Electrochemistry; Catalysis

Schedule:

Manuscript Submission Deadline: December 30, 2020

Peer Review Due: January 31, 2021

Revision Due: February 28, 2021

Announcement of Acceptance by the Guest Editors: March 10, 2021

Final Manuscript Due: March 25, 2021