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Full Schedule & My Itinerary

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Below is the full schedule for Pacifichem 2021. Within this page you can search for a Symposia Title, Presentation Title, and/or Presenter Name; and filter by Date, Topic Area, and Session Type. You can also change the preferred time zone so you can view in your own timezone (the default is Hawaii Standard Time).

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Advanced Filters

Filter by Date

Topic Area

Session Type

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Live Support

Preferred Time Zone

Eastern Standard Time (EST)

Event Itinerary

My Itinerary **2**

Analytical Development Relevant to Environmental Exposure and Effects (#27)

06:00pm - 10:00pm Eastern Standard Time (EST) - December 18, 2021 | Room: Virtual
Xing-Fang Li, Session Host; Prof. Dongchan Jang, Session Host
Topic Area: (01) Analytical
Session Type: Oral - Virtual

+ (https://pacifichem.digitellinc.com/pacifichem/rest/liveevents/itinerary)

Topic Area: (01) Analytical

Symposium Organizers: X. Li, S. Richardson, G. Jiang, S. F. Nakayama

Resolving identities of emerging per and polyfluoroalkyl substances isomers based on COSMO-RS derived retention factor and mass fragmentation patterns

Saturday

06:45pm - 07:15pm Eastern Standard Time (EST) - December 18, 2021 | Room: Virtual
Scott Simpson , Presenter; Mary Grace Guardian; Diana Aga
Topic Area: (01) Analytical
Session Type: Oral - Virtual

✕ (https://pacifichem.digitellinc.com/pacifichem/rest/liveevents/itinerary)

Hydrogen-rich systems: Materials chemistry for energy storage and delivery (#163)

01:00pm - 05:00pm Eastern Standard Time (EST) - December 21, 2021 | Room: Virtual
Godwin Severa, Session Host; Vitalie Stavila, Session Host
Topic Area: (12) Chemistry of Energy
Session Type: Oral - Virtual

+ (https://pacifichem.digitellinc.com/pacifichem/rest/liveevents/itinerary)

Topic Area: (12) Chemistry of Energy

Symposium Organizers: Z. Huang, M. Bowden, C. Yoon, T. HE, G. Severa

Tuesday

Search for molecular corks beyond carbon monoxide: A quantum mechanical study of N-heterocyclic carbene adsorption on Pd/Cu(111) and Pt/Cu(111) single atom alloys

04:05pm - 04:30pm Eastern Standard Time (EST) - December 21, 2021 | Room: Virtual

Scott Simpson , Presenter

Topic Area: (12) Chemistry of Energy

Session Type: Oral - Virtual

✖ (https://pacifichem.digitellinc.com/pacifichem/rest/liveevents/itinerary)

Periodic Density Functional Theory calculations reveal the potential application of 10 imidazole based N-heterocyclic carbenes to behave as “molecular corks” for hydrogen storage on single atom alloys, comprised of Pd/Cu(111) or Pt/Cu(111). Calculations show that functionalizing the NHC with different electron withdrawing/donating functional groups results in different binding energies of the NHC with the alloy surfaces. The results are compared to DFT calculations of carbon monoxide bound to these alloys. The Huynh electronic parameter (is calculated for several simple imidazole NHCs to gauge σ-donor ability, while Se-NMR of and P-NMR calculations of selenourea derivatives and carbene-phosphinidene adducts, respectively, have been utilized to gauge π-acidity of the NHCs. It is demonstrated that consideration of both σ and π donating/accepting ability must be considered when predicting the surface-adsorbate binding energy. It was found that electron withdrawing groups tend to weaken the NHC-surface interaction while electron withdrawing substituents tend to strengthen the interaction.