UNT HACKATHON SYMPOSIUM 23 August 2019

UNT EST. 1890

WHERE:

UNT Physics Building, Room 102. Reception at the Avesta Restaurant in the UNT Union.

WHEN:

August 23rd from 9:00 am to 5:00 pm.

PROGRAM:

8:30-9.00 AM: RECEPTION AND COFFEE

9:00 AM: **Jingbiao Cui** (Physics, UNT)
Welcome address

9.10 AM: **Oliviero Andreussi** (Physics, UNT)
"UNT HACKATHON: summary and perspectives"

9:35 AM: **Tom Cundari** (Chemistry, UNT)
"New Strategies for an Old Problem: Methane Activation"

10:00 AM: **Michele Pavanello** (Physics, Rutgers)
"Density Embedding Methods for the Condensed Phase"

10:25 AM: COFFEE BREAK

10:40 AM: **Jason Goodpaster** (Chem., Minnesota)
"Quantum embedding and machine learning for complicated electronic structure systems"

11:10 AM: **Kyeongjae (KJ) Cho** (Materials, UTD)
"TDDFT Modeling of Electron-Enhanced Atomic Layer Deposition"

11:40 AM: **Sehr Naseem Khan** (Chemistry, UNT)
"Water: Only three atoms but a challenge for polarizable force field developers"

12:00 PM: **Jagoda Slawinska** (Physics, UNT)
"Tuning of spin Hall effect in two-dimensional monochalcogenides"

12:20 PM: LUNCH @ AVESTA

1:20 PM: **Hao Yan** (Chemistry, UNT)
"Computational chemistry under extreme mechanical conditions"

1:50 PM: **Muhammad Huda** (Physics, UTA)
"Formation of polarons, their electronic structures and effects in metal-oxide-photoelectrocatalysts"

2:20 PM: **Jincheng Du** (Materials, UNT)
"Glass genome: from atomistic simulations to QSPR analysis of inorganic glasses"

2:50 PM**: Andrew Baczewski** (Sandia)
"X-ray Thomson scattering in warm dense matter using time-dependent density functional theory"

3:15 PM: COFFEE BREAK

3:30 PM: **Elfi Kraka** (Chemistry, SMU)
"Solving Chemical Problems on SMU's High-Performance Computer ManeFrame II"

4:00 PM: **Kwangho Nam** (Chemistry, UTA)
"Chemo-Mechanical Coupling of F1-ATPase: Insights from Molecular Simulations"

4:30 PM: **Qiming Zhang** (Physics, UTA)
"Tunable piezoelectricity of the alkali niobate-based ceramics"

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ORGANIZING COMMITTEE:

Oliviero Andreussi, G. Andrés Cisneros, Marco Buongiorno Nardelli

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