



Dear Colleagues,

I am happy to share the Fall 2024 O'Donnell

Dr. Corey Clark, SMU Guildhall

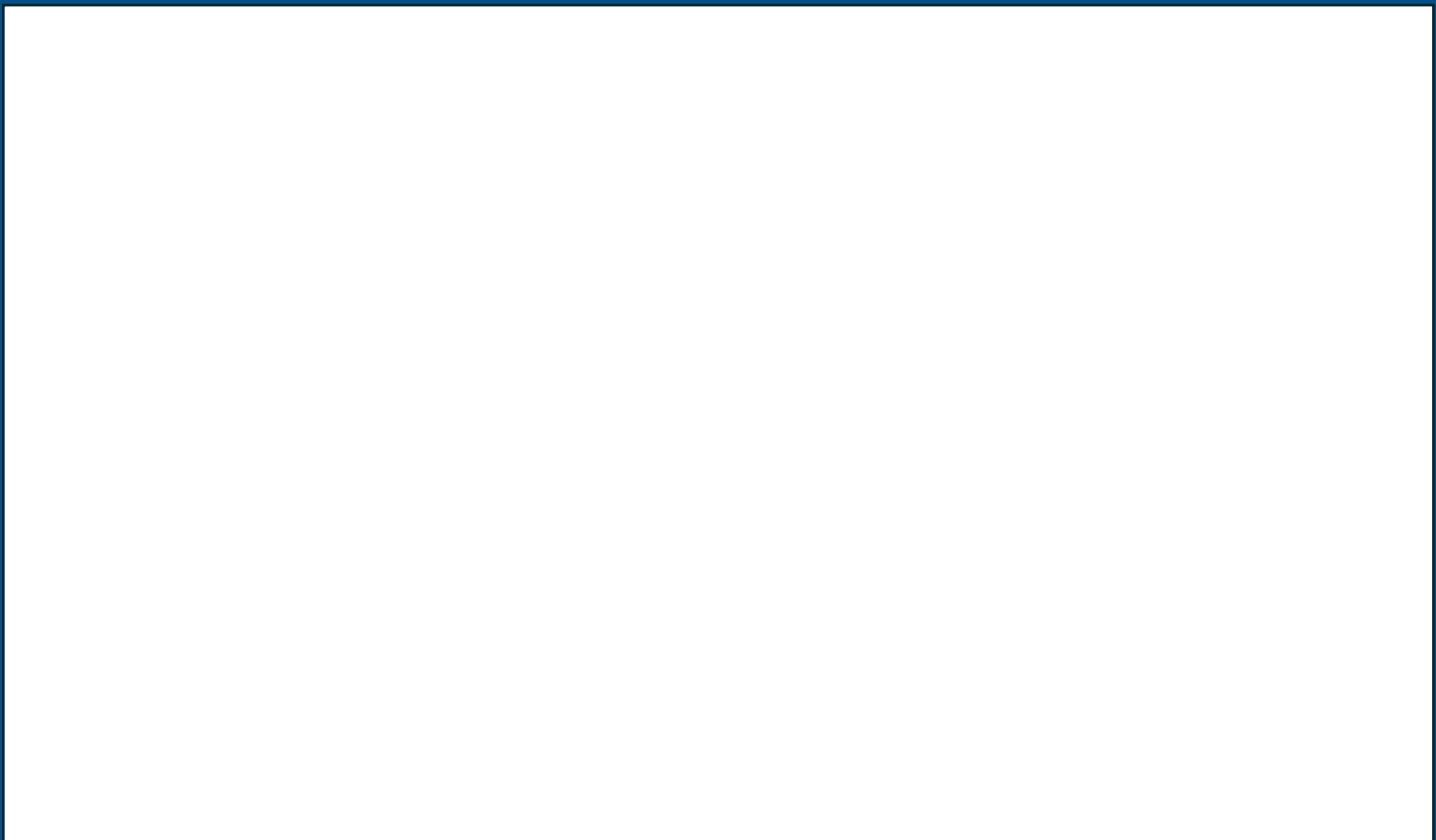
---

When appropriate learning materials are accessible, students with reading disabilities can effectively demonstrate their understanding in ways comparable to their peers. AI agents, powered by Large Language Models (LLMs), present a unique solution for providing universal access to students with reading disabilities by offering personalized learning experiences tailored to individual needs. This personalization enhances learning without compromising the generalizability of the AI agents' design, allowing a single agent design to adapt to diverse scenarios. Dr. Clark's research aims to advance AI agent design and deploy these agents in middle school classrooms to promote equity and better prepare students for technology-driven careers. These AI agents will also support teachers by offering data-driven insights into student progress, making it easier to track and address diverse learning needs. This research integrates game-based AI agents—driven by LLMs—into an educational version of Minecraft to personalize learning experiences, discover optimal metrics for supporting students with reading disabilities, and provide teachers with summaries and analytics on student progress. The AI agents are divided into two types: Personalized Education Agents and Teacher Support Agents. Integrated into Minecraft, these agents assist students through personalized feedback and game scenarios tailored to their reading needs, while helping teachers understand student progress through accessible summaries and visualizations.

Dr. Mehak Gupta, Computer Science

---

Dr. Mehak Gupta's research team has made a significant breakthrough in harnessing the power of Artificial Intelligence (AI) for psychological assessments, leveraging cutting-edge Natural Language Processing (NLP) techniques to enhance technical





Dr. Elf Kraka, Chemistry; Dr. Corey Clark, SMU Guildhall

---

The Computational and Theoretical Chemistry Group (CATCO) at SMU, led by Dr. Elf Kraka, is dedicated to developing innovative quantum chemical tools that can accelerate chemical discovery processes, reduce the need for costly and dangerous experiments, and provide insights not accessible through traditional methods. In addition to advancing scientific knowledge, CATCO is committed to educating and mentoring graduate students and postdoctoral researchers to become the next generation of leaders in their field. Recently, CATCO has joined forces with Dr. Corey Clark's Guildhall Human and Machine Intelligence (HuMI) Game Lab to develop a novel drug design platform that combines the power of Artificial Intelligence (AI) and Quantum Mechanics (QM).

This interdisciplinary collaboration has already yielded significant results, including the creation of SmartCADD, a user-friendly virtual screening platform for drug discovery that can efficiently screen billions of compounds and identify potential leads. In a pilot study, SmartCADD successfully









