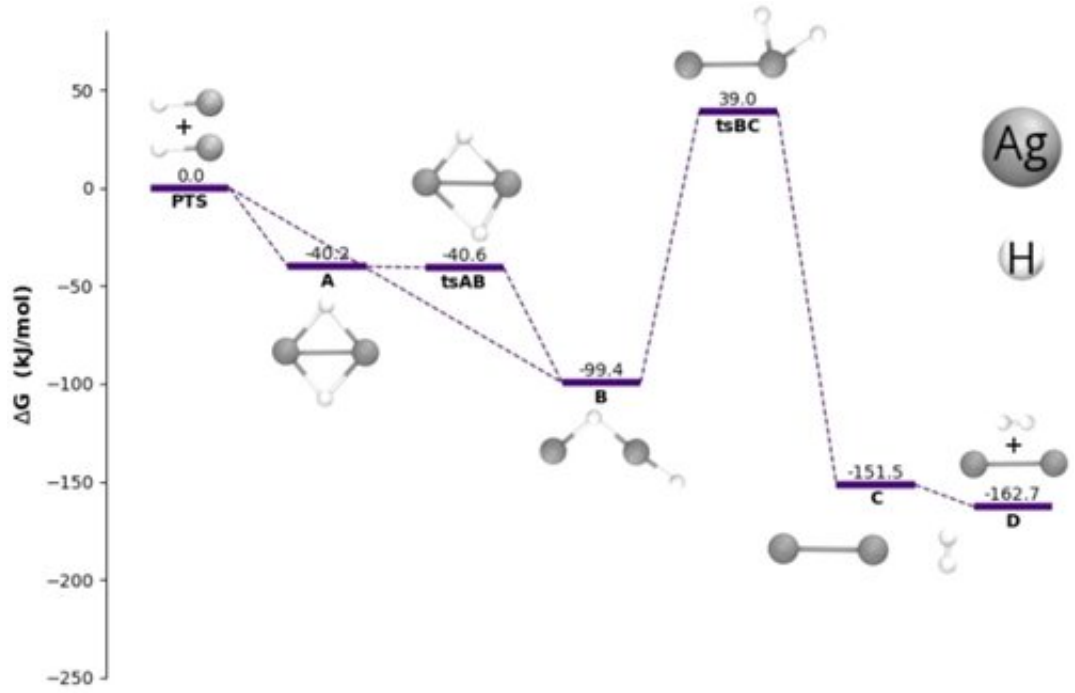
Quantum chemists conjure recipe to turn gold, silver and copper into vessels of green energy

September 8 2021



Free energy profile for the reaction involving AgH monomers. D corresponds to the Ag2 and H2 molecules at the dissociation limit. All the free energies (in kJ · mol−1) were obtained at MP2/aug-cc-pVQZ//aug-cc-pVTZ. Credit: DOI: 10.1002/open.202100108

Quantum chemists believe gold, silver and copper could help the world take a leap towards green energy after discovering that compounds based

on these metal elements and hydrogen are very promising candidates for hydrogen storage.

These "metal hydride" complexes could be used to store hydrogen for use on board vehicles, for example, where it must be stored cryogenically and/or at very high pressure.

Hydrogen is volatile at ambient temperature, which is why scientists have paid particular attention to the design of low-cost materials that can reversibly and rapidly store it for use in everyday situations.

Metal hydride research has been focused on improving the storage capacity of such materials for some time, making the newest discovery—just published in leading journal *Chemistry Open*—even more exciting.

Dr. Cristina Trujillo, Research Fellow in Trinity College Dublin's School of Chemistry, and based in the Trinity Biomedical Sciences Institute, is the senior author of the journal article. She said:

"Among the greatest challenges facing humanity is the growing need to stop global warming and find more efficient and cleaner ways to produce energy. As everybody already knows the current production system and excessive use of fossil fuels is releasing much more CO_2 into the atmosphere than is being absorbed naturally, which makes the creation of greener and more environmentally friendly alternatives a global priority.

"For decades now many research groups across the world have put their efforts into this issue. One of the most studied alternatives has been hydrogen as a clean and CO_2-free energy source, but it presents multiple problems due to its reactivity, and low density and stability.

"Our contribution here—made via quantum chemistry techniques—has been to show that gold, silver and copper hydride complexes are very likely to effectively retain hydrogen in a stable manner. We hope that this work will have multiple applications in time to come."

The Trinity team of Dr. Trujillo and Ph.D. Candidate, Inigo Iribarren, has been collaborating with Professors Ibon Alkorta and Jose Elguero (IQM-CSIC, Spain) and Dr. Sánchez-Sanz (Irish Centre for High-End Computing, Dublin) on various compound-bonding interactions for years.

Recently the team has been investigating "regium bonds" in great detail. Regium bonds have shown great promise in understanding how metals interact with other chemical species, ultimately leading the team to look at gold and silver complexes as potential ingredients for a recipe that could make a global difference in a more sustainable future.

More information: Iñigo Iribarren et al, Reactivity of Coinage Metal Hydrides for the Production of H 2 Molecules, *ChemistryOpen* (2021). DOI: 10.1002/open.202100108

Provided by Trinity College Dublin