One of the main drawbacks of metallic glasses is their low thermodynamic stability, which limits their formability and service life. Recently, experiments by members of the Wisconsin MRSEC showed that organic glasses with high thermodynamic stability can be synthesized via physical vapor deposition (PVD) onto a substrate at a controlled temperature. Now, this team of researchers has used molecular dynamics simulations to predict that the same PVD methods can enhance the stability of metallic glasses (top figure).

Simulated metallic PVD glasses (Zr44Cu50Al6) have a lower potential energy than melt-quenched glasses with the same composition (bottom figure), which means that the PVD metallic glasses are more stable. Simulations also provide atomistic insight into the mechanisms for enhanced stability: compared to the melt quenched glass, the PVD glasses have more homonuclear bonds and therefore are more chemically ordered. To achieve the stability of the PVD metallic glass by melt quenching would require a cooling rate 4 orders of magnitudes slower than the typical cooling rates used melt quenching (which is not accessible by normal means).