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Structural isomerism in gold nanoparticles revealed by X-ray crystallography

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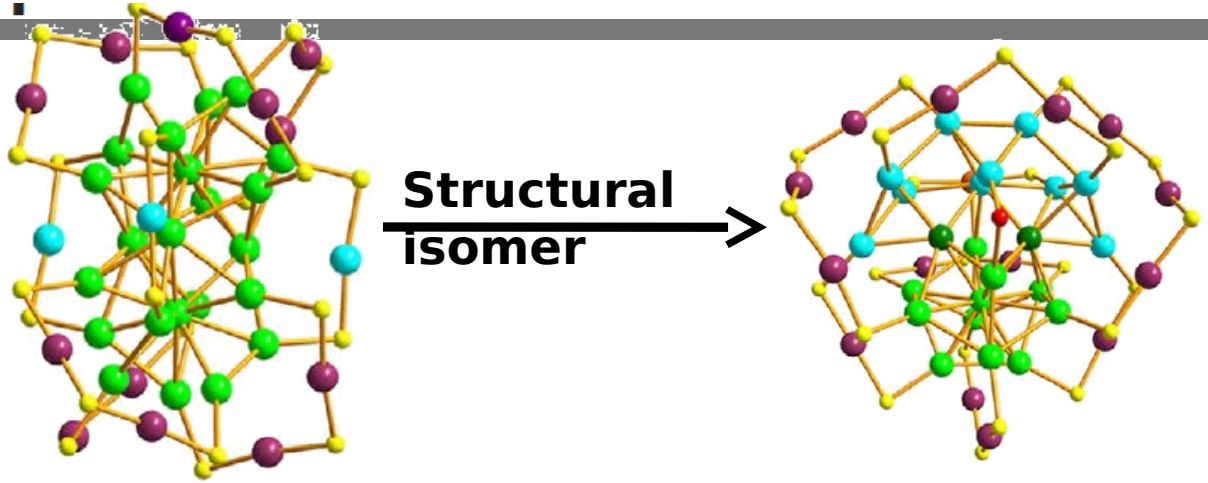

Background....

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Total Structure Determination of Thiolate-Protected Au_{38} Nanoparticles

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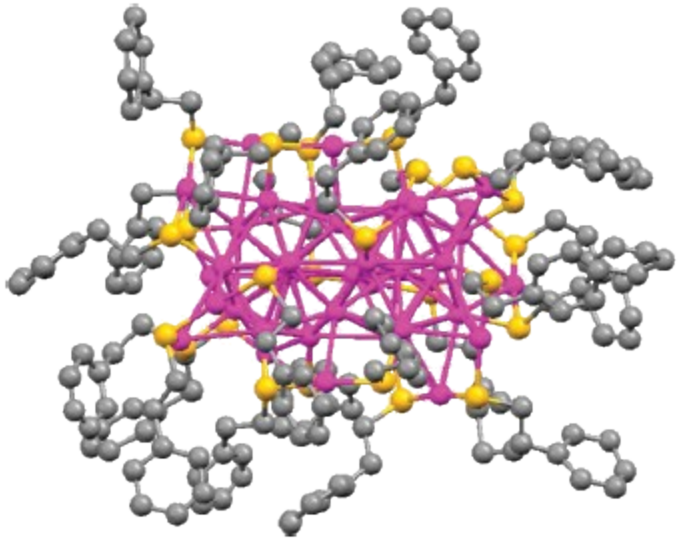
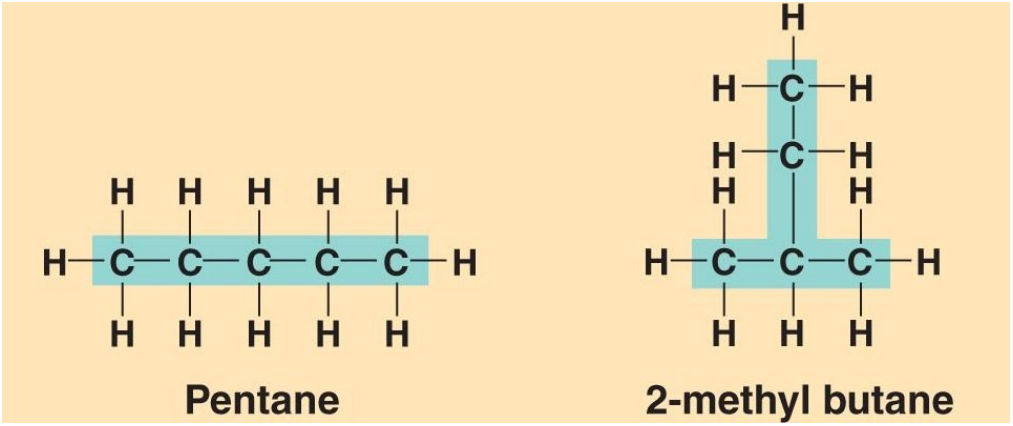


Structural isomerism



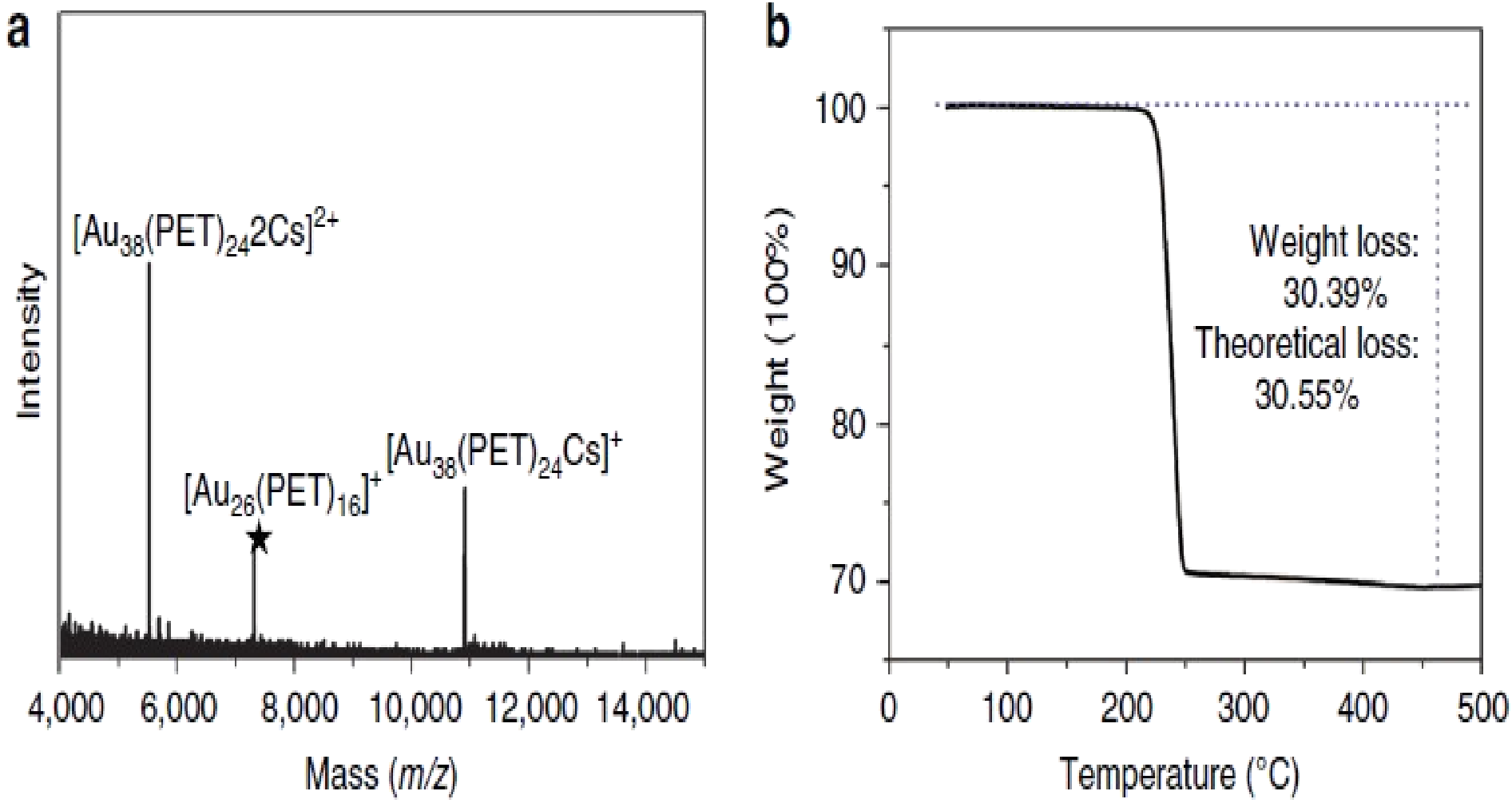
• Structural isomerism at nanoscale.

• Resolving structure reveals structure property correlation and guidance for synthesizing functional material.

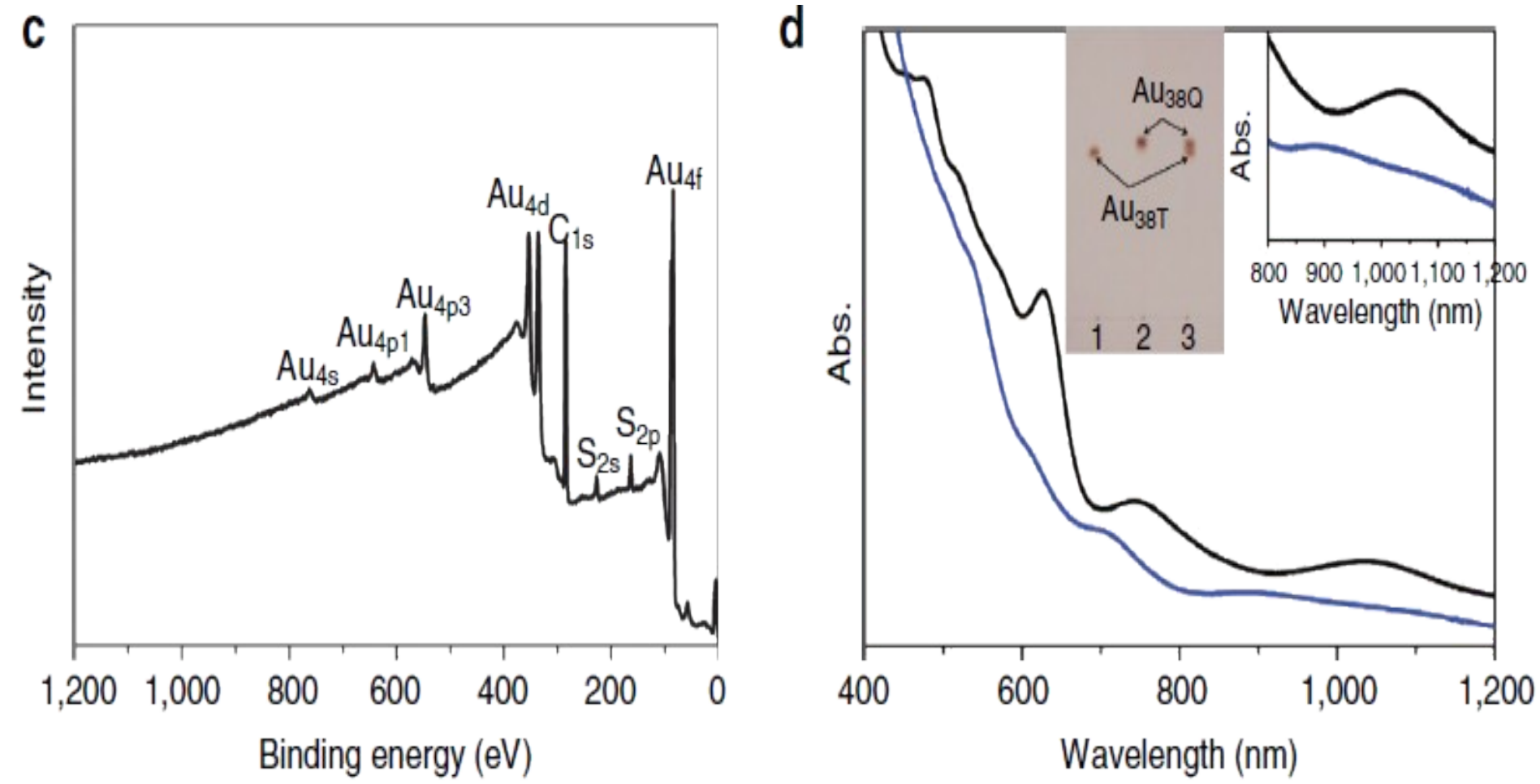
• $Au_{24}(SCH2Ph\text{-}tBu)_{20}$ and $Au_{24}(SePh)_{20}$ have different Au24 core structures.

Synthesis of $Au_{38}PET_{24}$ → PTLC, ESI-MS, TGA, XPS → Single crystal X-Ray crystallography(SCXC)

Au_{38T} (new)-Tian —50°C→ Au_{38Q} (old)-Qian

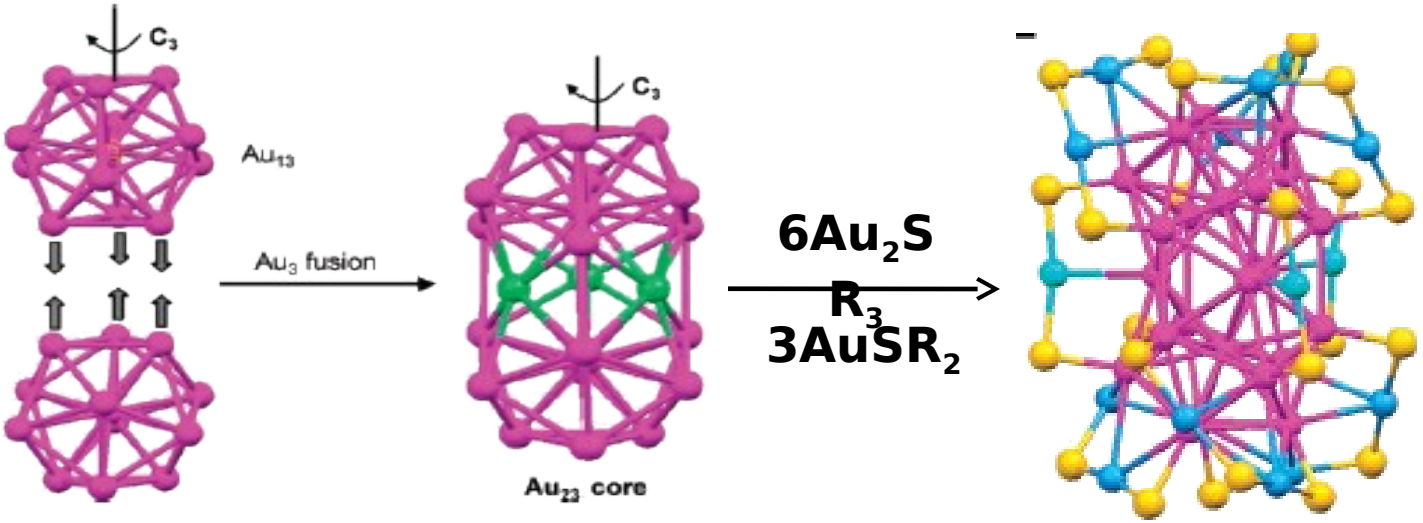


(a) ESI mass spectrum of the Au_{38T}. (b) TGA of Au_{38T}.

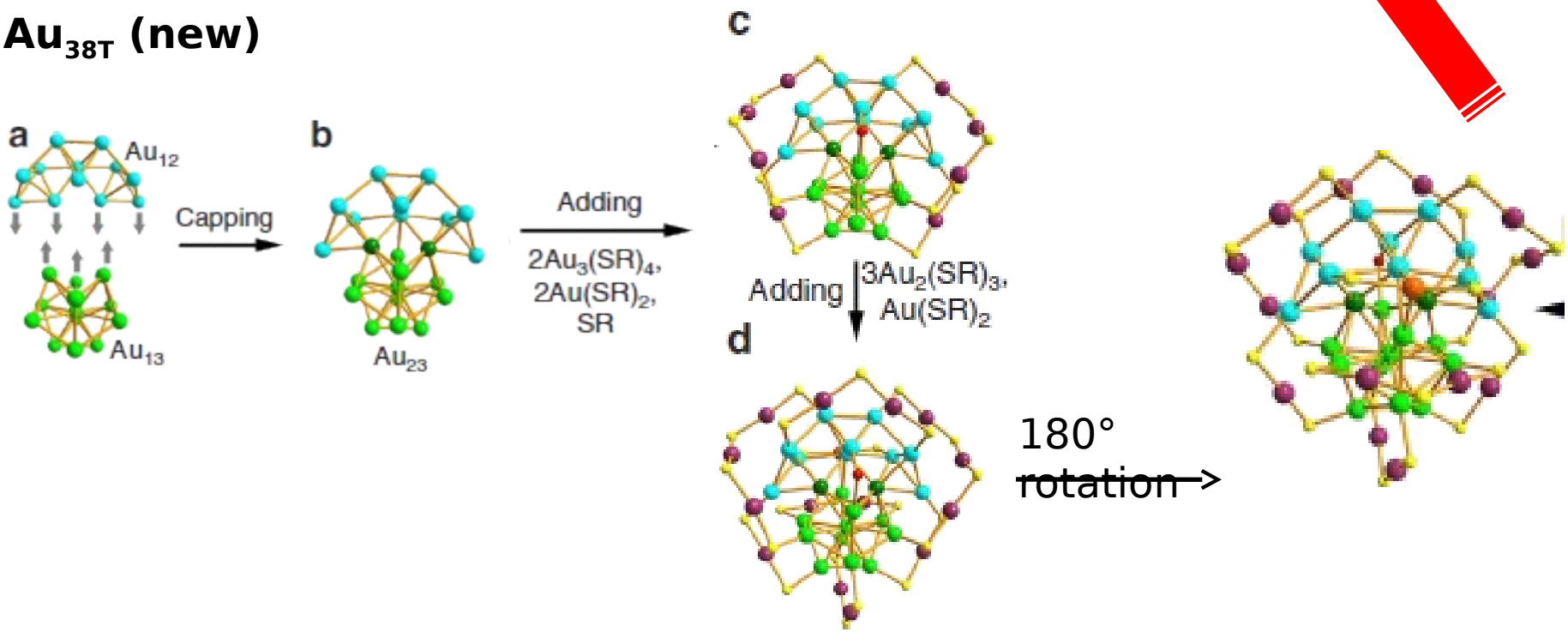


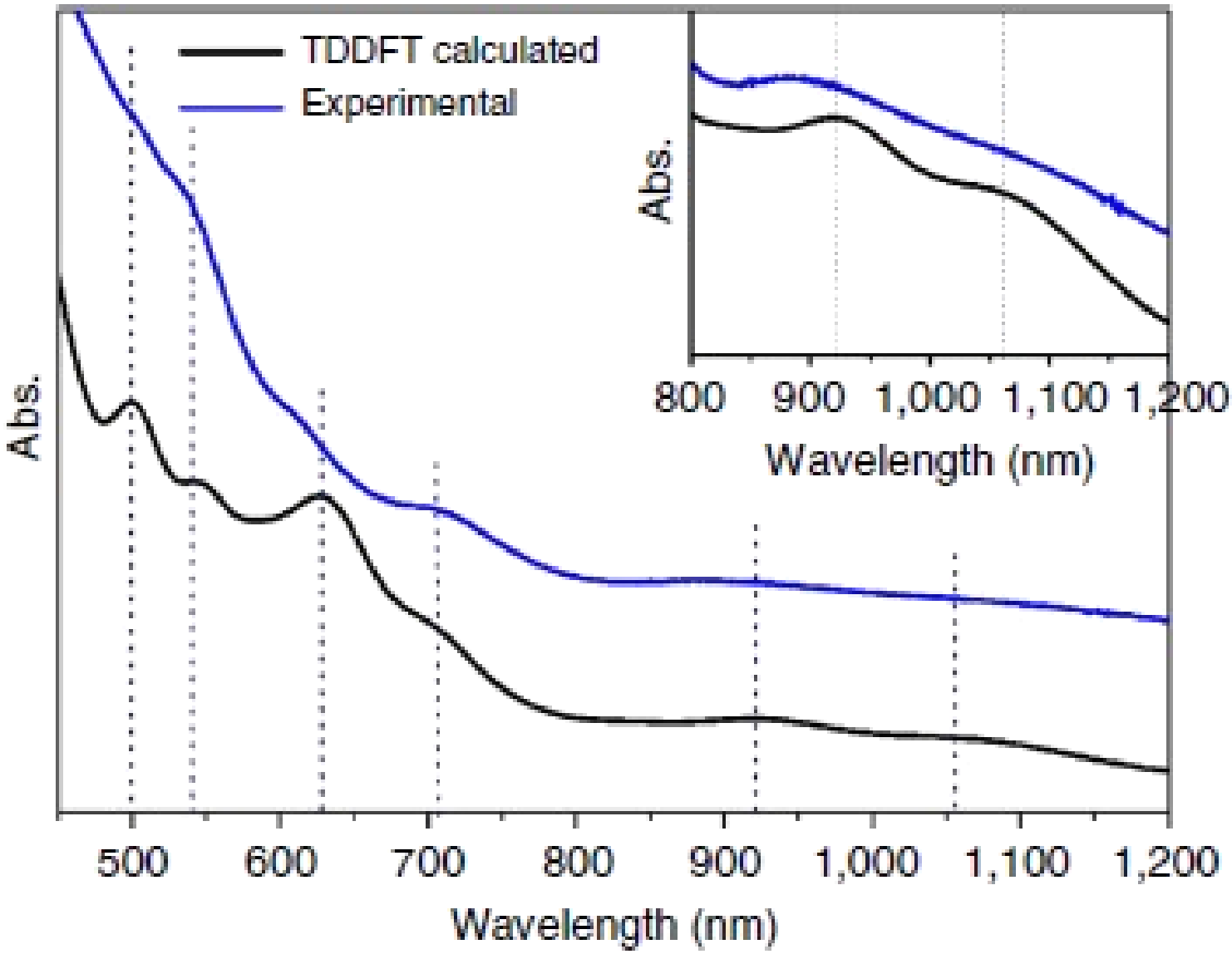
(c) XPS spectrum of Au_{38T}. (d) Ultraviolet–visible–near-infrared absorption spectra of Au_{38T} (blue) and Au_{38Q} (black) in toluene (measurement temperature: 0° C). Insets are the photo of thin-layer chromatography and enlarged absorption spectra in the range from 800 to 1,200nm of Au_{38T} and Au_{38Q}.

Au_{38Q} (old)

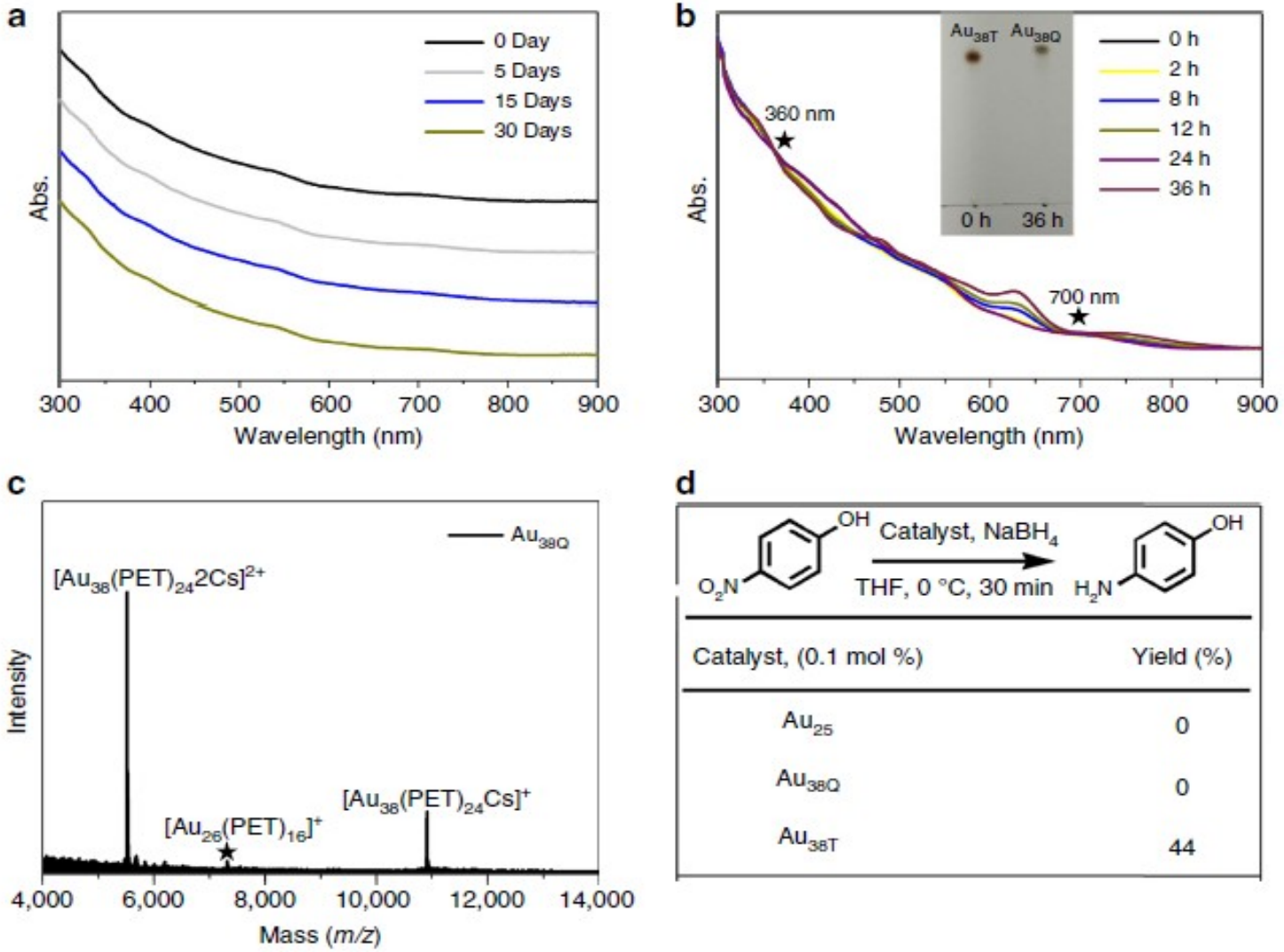


Au_{38T} (new)





Comparison of ultraviolet–visible–near-infrared absorption spectra of Au38T. Blue: experimental; black: calculated by time-dependent density function (TDDFT) method. Inset is the enlarged spectra in the range from 800 to 1,200 nm.



(a) Time-dependent ultraviolet–visible–near-infrared absorption spectra of Au_{38T} at -10°C in toluene. (b) Ultraviolet–visible–near-infrared absorption spectral transformation at 50°C in toluene (the isosbestic points are at 360 and 700 nm). Inset: thin-layer chromatography of Au_{38T} before and after the transformation. (c) ESI mass spectrum of the transformed product

Conclusion

• A novel synthesis method is developed, with which a novel gold nanoparticle readily
synthesized, and the composition of the as-prepared nanoparticleis precisely determined using
ESI–MS in conjunction with XPS and TGA.

• The structure of Au38T is resolved using SCXC and the unique structural features provide important implications for nanocluster structural studies.

• Significantly, structural isomerism is observed in nanoparticles for the first time.

• The distinctly different properties (in particular the catalytic properties) of the two structural isomers indicate a structure–property correlation and this will have important implications for
future catalytic studies.

Future directions.

HPLC separation of clusters is a very new field.

Finding suitable eluents and column for ligand exchanged products, chiral mixtures and other isomers will lead to efficient separation.

PAPER

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Separation of carbon quantum dots on a C18 column by binary gradient elution *via* HPLC†

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Carbon quantum dots (CQDs) have attracted significant attention due to their low toxicity, biocompatibility and potential applications, particularly in the field of biomedical imaging. However, the major drawback limiting the application of CQDs is their relatively low quantum yield (QY). For further study and applications of CQDs, this class of carbon nanomaterials requires separation and purification. In this paper, we report a general method to separate CQDs obtained using resorcinol (*m*-$C_6H_6O_2$) as the carbon precursor on a C18 column through high performance liquid chromatography (HPLC). The separation of CQDs was achieved by binary gradient elution using acetonitrile–water and acetonitrile–methanol as the mobile phases and acetonitrile plays an important role in the separation of CQDs. The resolution of some peaks improved when the flow rate was increased; however, the separation of certain other peaks worsened, almost disappearing at higher flow rates. The characterization of the collected fractions revealed that the oxygen-containing functional groups on the CQDs are crucial when separating the CQDs through this method. Our method is feasible and the collected purified CQDs have QY as high as 0.72.

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THANK YOU