Supplementary Information: Thiol Click Chemistry on Gold-Decorated MoS₂: Elastomer Composites and Structural Phase Transitions

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Figure S1. AFM image of as-exfoliated MoS₂ flakes. The color code bar contains a height histogram showing two main peaks ascribed to the substrate and the flakes. Detailed XPS spectra of Au 4f (b), Mo 3d and S 2s (c), and S 2p (d) signals of lithium intercalated and exfoliated MoS₂, undecorated (red) and gold decorated (blue) samples.

The exfoliated flakes have typical lateral sizes of a few 100 nm (Fig. S1a) and uniform thicknesses of 1.7 nm. While mechanical exfoliation yields step heights of 0.7 nm, consistent with the crystal structure of MoS₂, chemical exfoliation typically yields monolayers with thicknesses exceeding 1 nm.¹ This discrepancy may be explained by surface corrugation due to distortions as well as adsorbed or trapped molecules. The AFM height profile shows that all flakes have the same thickness and no steps, suggesting they all have the same number of layers.

The XPS spectra of as-exfoliated (undecorated) and gold-decorated flakes are shown in Figs. S1b-d. While the as-exfoliated sample shows sulphur only in the oxidation state S^{2-} , upon GNP decoration some of the sulphur is oxidized to S^{4+} and/or S^{6+} . Additionally, the decorated flakes show a gold doublet Au 4f spectrum (Fig S1b), which points towards a significant presence of both gold atoms bound to sulphur in the flakes and gold atoms bound only to other gold atoms within a GNP. These results confirm the invoked nucleation of GNPs proceeding via the reduction of HAuCl₄ and oxidation of MoS₂.

1 G. Eda, H. Yamaguchi, D. Voiry, T. Fujita, M. Chen and M. Chhowalla, *Nano Lett.* 2011, **11**, 5111.

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