Table 4. Calculated harmonic frequencies (cm^{-1}) for the models proposed systems. In parenthesis is the force constant (mdyne/Å).

System	Method	ν (S-Au)	ν(S-H)	ν (S-H)
$C_8H_{17}SH$	MP2		836 (0.531)	2824 (4.879)
	PBE-D3		699 (0.587)	2592 (4.116)
	Exp [54]		655	2740
$C_8H_{17}SH-[Au]_4$	MP2	358 (0.932)	636 (0.263)	2734 (4.571)
	PBE-D3	303 (0.221)	675 (0.928)	2548 (3.977)
2α-CD/$C_8H_{17}SH$	MP2		644 (0.501)	2622 (4.003)
	PBE-D3		663 (0.526)	2519 (4.120)
	Exp [57]		613	2573
2α-CD/$C_8H_{17}SH-[Au]_4$	PBE-D3	303 (0.220)	651 (0.492)	2366 (3.439)
2α-CD/$C_8H_{17}SH-[AuNP]$	Exp [56]	312	605	2580

4. CONCLUSIONS

This work provides new insights into the rational design and characterization of solid materials by a theoretical point of view. The Au-S interaction in the interface and an exhaustive chemical structure of a solid phase material was described by ab-initio and DFT calculations. The self-assembly is mediated by –SH functional groups, located outside the host-guest complex, evidenced through Au-S and S-H vibrational modes. Theoretical calculations allow for determination of the magnitude of the Au-S interaction, where the correlation energy plays an important role in the system stability. The theoretical results confirm that van der Waals forces predominate in the neutral systems. The estimated vibrational frequencies for Au-S and S-H are in good agreement with results obtained by vibrational and Raman spectroscopy. As a perspective, these results suggest the importance of knowing in detail the interface of Au-S systems in the solid phase for the development of new highly efficient materials in practical applications.

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