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THE SERS ANALYSIS OF THE INTERACTION BETWEEN Ag_8 CLUSTER AND ADENINE FOR OPTICAL SENSOR APPLICATIONS USING DFT CALCULATIONS

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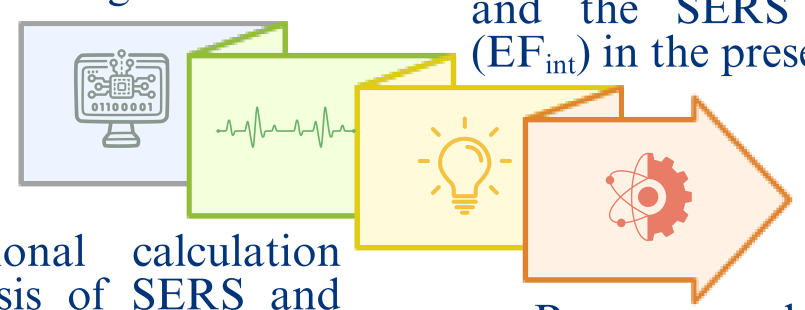
INTRODUCTION & AIM



Determine the optimal excitation wavelength

Characteristic vibrations of adenine and the SERS enhancement factor (EF_{int}) in the presence of Ag_8 clusters

Computational calculation and analysis of SERS and Raman spectra

Propose a basis for wavelength and characteristic vibrational in adenine detection toward label-free silver cluster biosensors

METHOD

Computational details

- DFT
- DFT Functional: PBE0
- Basic set: Def2-TZVP
- Solvation model: IEF-PCM (water)

Guassian 16

Multiwfn 3.8

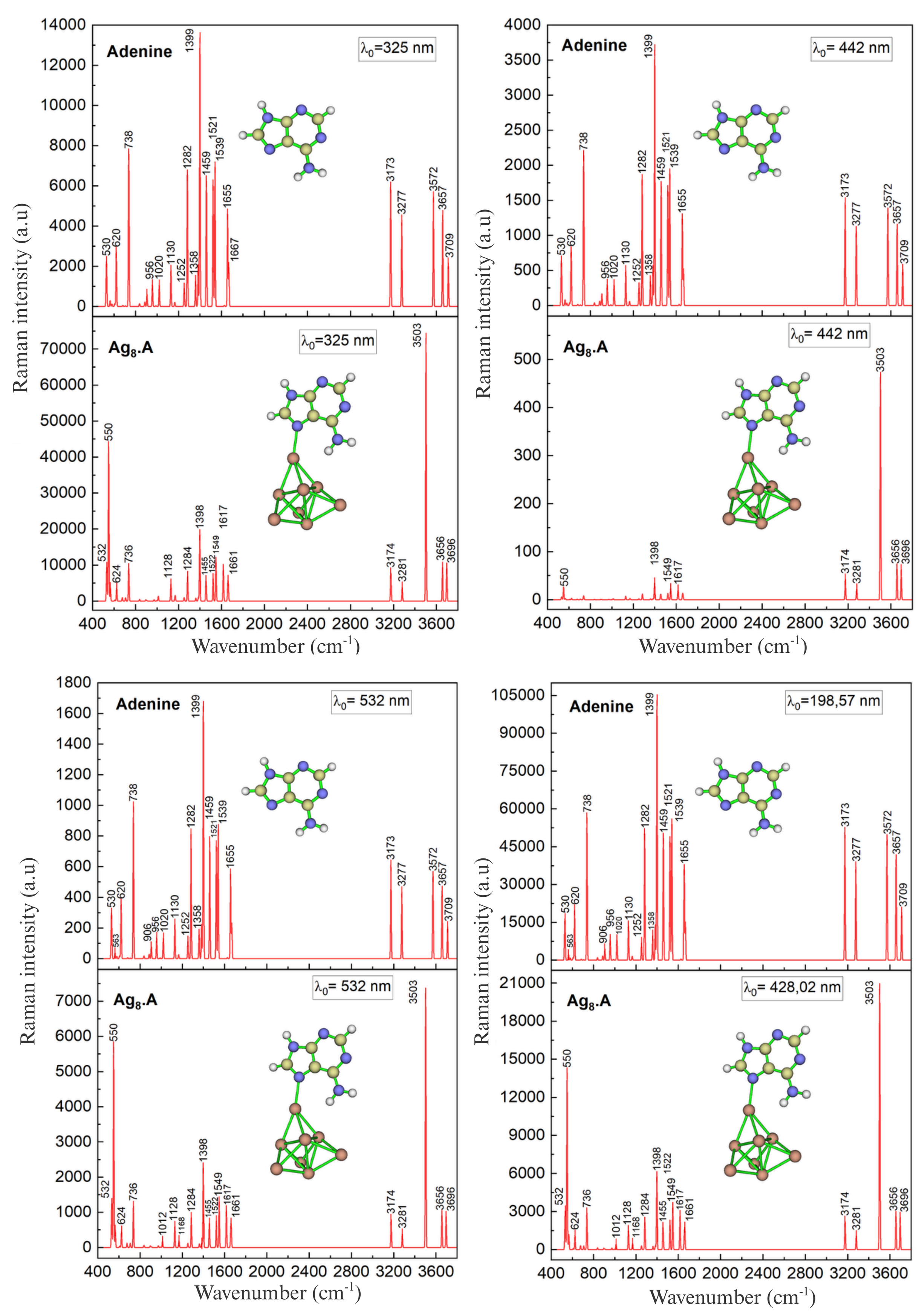
RESULTS & DISCUSSION

Time-Dependent Density Functional Theory

Matter	E_{exc} (eV)	λ_0 (nm)	f
Adenine	5,019	247,03	0,463
	6,244	198,57	0,62
Ag_8•A	2,3	539,01	0,547
	2,803	442,37	0,915
	2,897	428,02	1,482
	3,869	320,5	0,003

Analysis of the Raman spectrum of adenine and the SERS spectrum of Ag_8•A

Excitation wavelength near calculated value

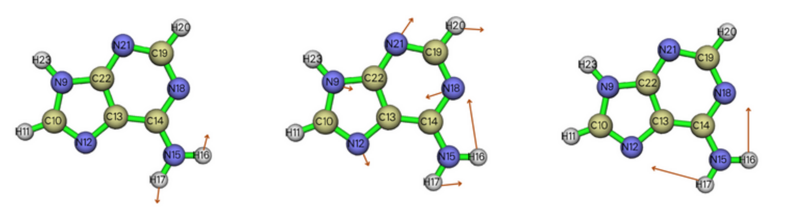


Raman spectrum of adenine (top) and SERS spectrum of Ag_8•A (bottom) at different excitation wavelengths.

Characteristic vibrations of adenine

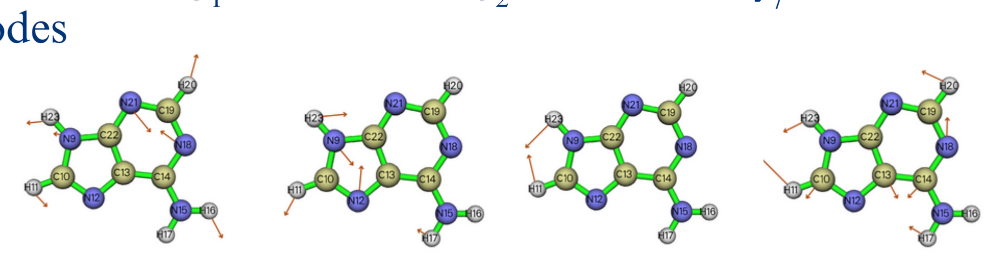
Symbol	Vibrations	Raman Adenine		SERS Ag_8•A		EF_{int}
		n	R_i	n	R_i	
ν_1	ω (NH_2)	580 (534[d])	0,6 (0[d])	550	223,4	359,1
ν_2	ρ (NH_2), ρ (CH), φ_6	620 (621[a], 618[b])	16,3	624 (689[c])	21,3	1,3
ν_3	γ_6(CH)	906 (904[b])	5,8	907	1,4	0,3
ν_4	ν_{b5}	956 (949[b])	10,9	972 (950[c])	3,8	0,4
ν_5	σ_5 (NH, CH)	1130 (1127[b])	22,4	1128 (1190[c])	58,9	2,6
ν_6	σ_5 (NH, CH), ρ_6 (CH)	1399 (1397[d])	217,1 (27[d])	1398 (1392[d])	295,8 (38[d])	1,4
ν_7	σ (NH_2)	1626 (1596[d])	1	1617	164,9	163,9
ν_8	ν_{as6} (C-H)	3173 (3160[b], 3111[d])	276,7 (120[d])	3174	368,6	1,3
ν_9	ν_{as5} (C-H)	3277 (3269[b])	210,3	3281	186,4	0,9
ν_{10}	ν_s (H-N-H)	3572 (3433[b], 3451[d])	306,0 (174[d])	3503	3992,6	13
ν_{11}	ν_{as5} (N-H)	3657 (3497[d])	260,7 (144[d])	3656	536	2,1
ν_{12}	ν_{as} (H-N-H)	3709 (3550[b], 3587[d])	128,3 (46[d])	3696	533,1	4,2

NH_2 vibrations



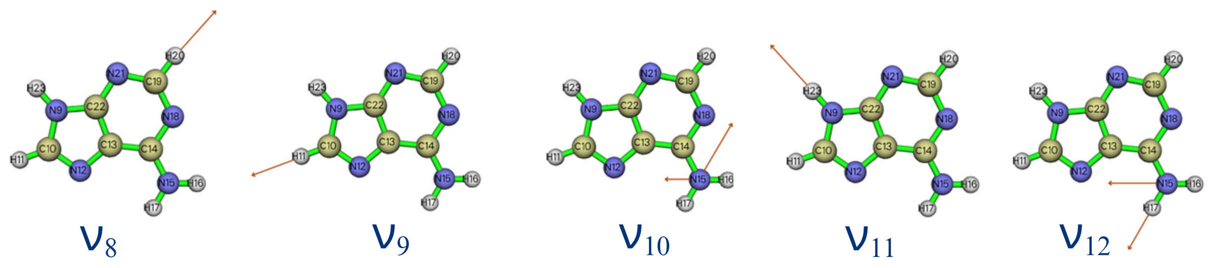
ν_1 ν_2 ν_7

Ring vibrational modes



ν_3 ν_4 ν_5 ν_6

C–H and N–H stretching vibrations



ν_8 ν_9 ν_{10} ν_{11} ν_{12}

CONCLUSION

- Among the excitation wavelengths investigated, the 325 nm wavelength provides the greatest signal enhancement and yields the most characteristic vibrational peaks;
- The results identified the characteristic vibrational modes of adenine.
- The study demonstrated that Ag_8 induces a pronounced enhancement of the Raman signal of adenine, with the resulting enhancement factor exceeding those reported in previous studies.

FUTURE WORK / REFERENCES

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