Revised Manuscript ID: CP-ART-10-2012-043511

Supporting information

Molecular Reactivity Dynamics in a Confined Environment

Munmun Khatua[a] and Pratim Kumar Chattaraj*[a]

[a]Department of Chemistry and Center for Theoretical Studies,

Indian Institute of Technology Kharagpur,

Kharagpur 721302, West Bengal, India.

*Author for correspondence: email : pkc@chem.iitkgp.ernet.in

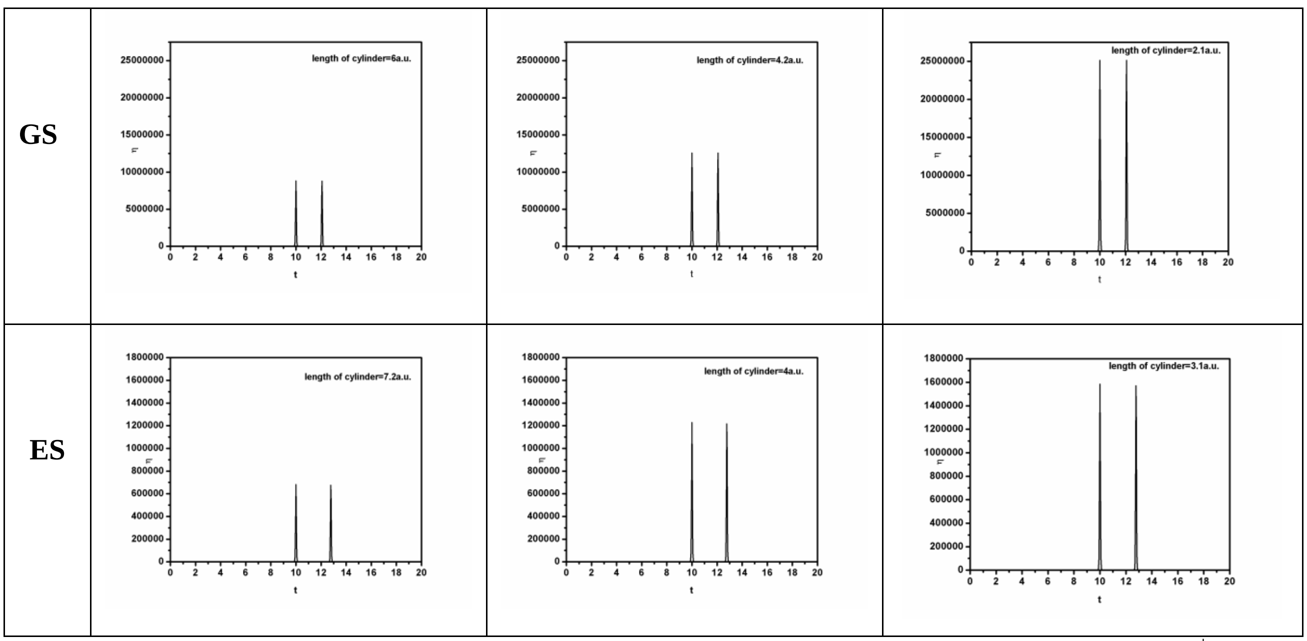


Figure S1: Time evolution of chemical hardness (η) during a collision process between H^+ and N_2 molecule in ground state (GS) and excited state (ES) in a confined environment (length of cylinder = 6.0a.u. denotes unconfined system in GS and 7.2a.u. in ES).

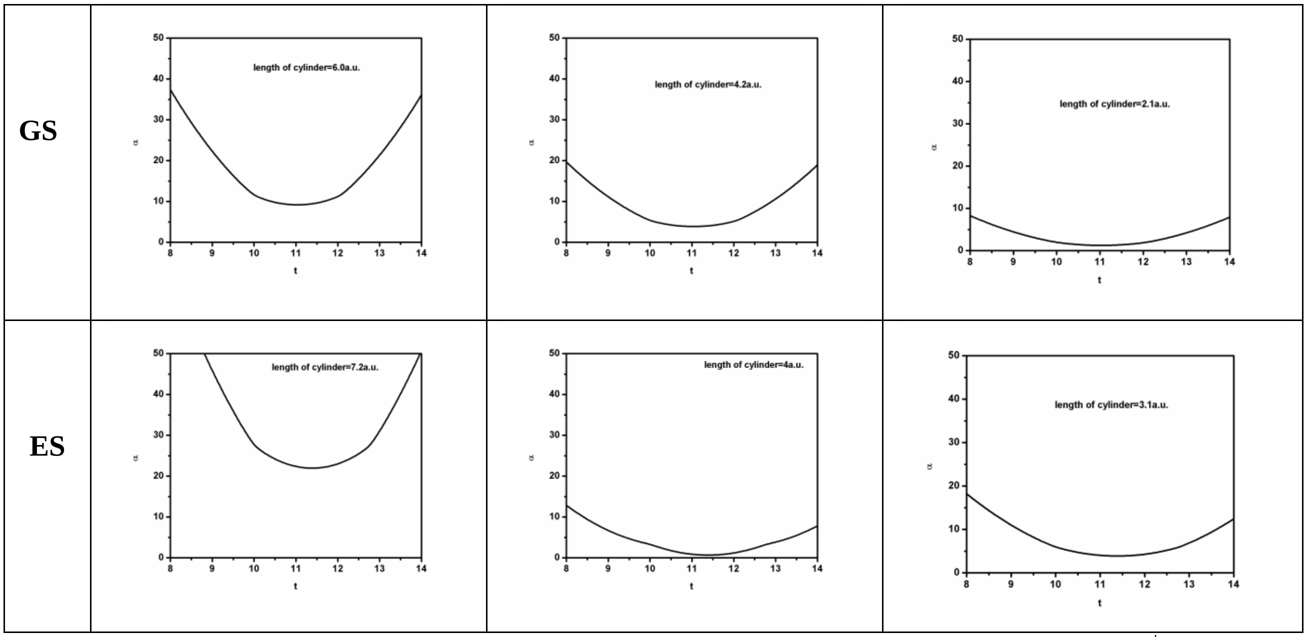


Figure S2: Time evolution of polarizability (α) during a collision process between H^+ and N_2 molecule in ground state (GS) and excited state (ES) in a confined environment (length of cylinder = 6.0a.u. denotes unconfined system in GS and 7.2a.u. in ES).

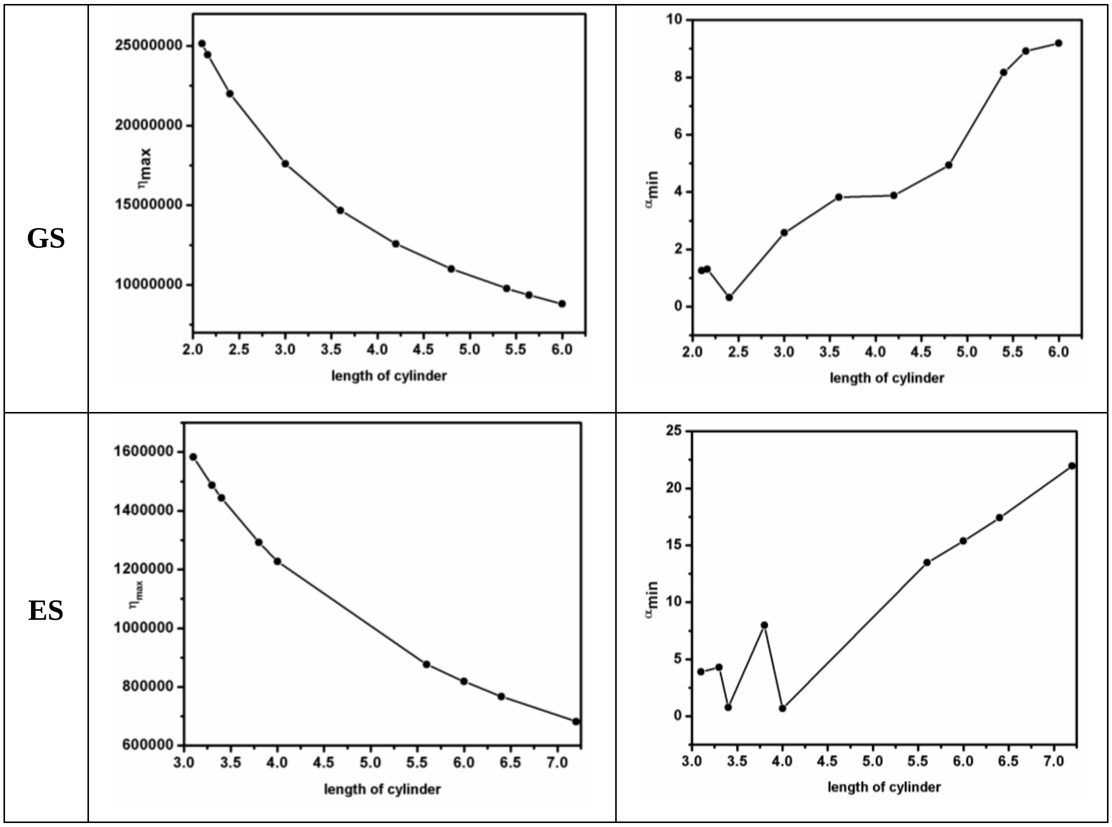


Figure S3: Plots of η_{max} vs. length of cylinder and α_{min} vs. length of cylinder during a collision process between H^+ and N_2 molecule in GS and ES.

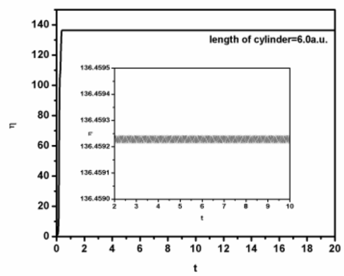
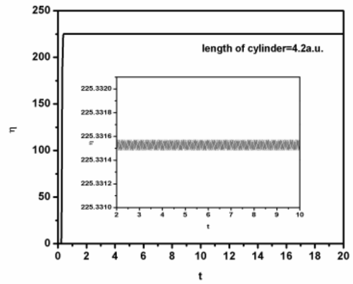
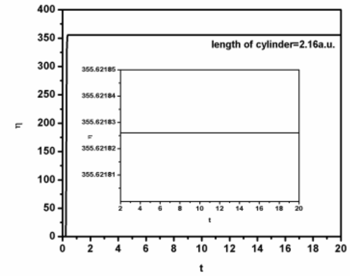
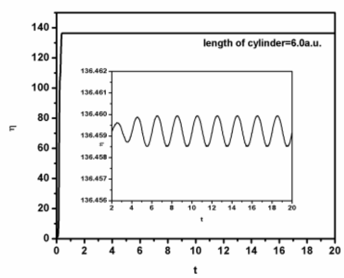
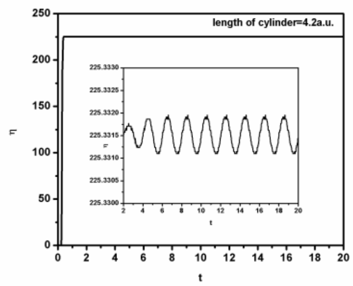
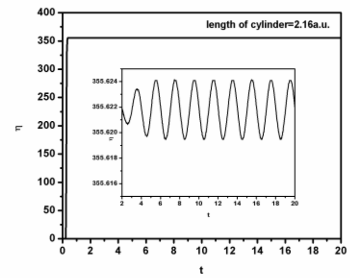
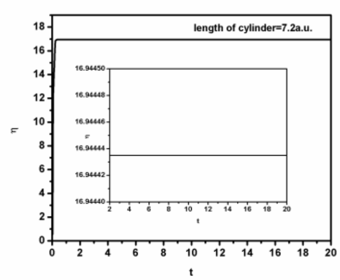
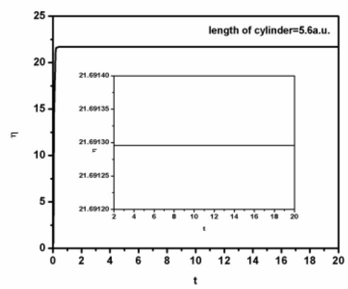
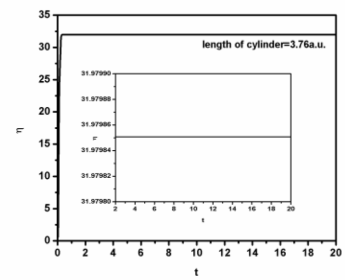
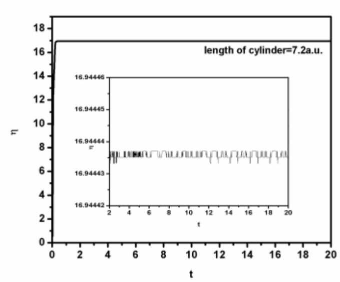
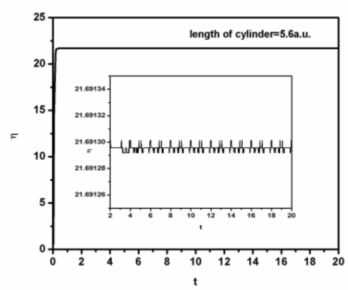
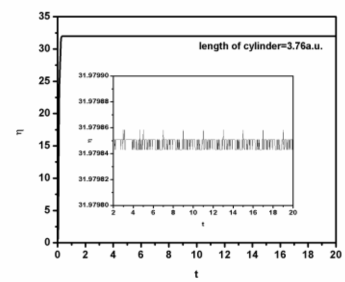
GS	ε_0=0.01			
	ε_0=100			
ES.	ε_0=0.01			
	ε_0=100			

Figure S4: Time evolution of chemical hardness (η) when N_2 molecule in ground state (GS) and first excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

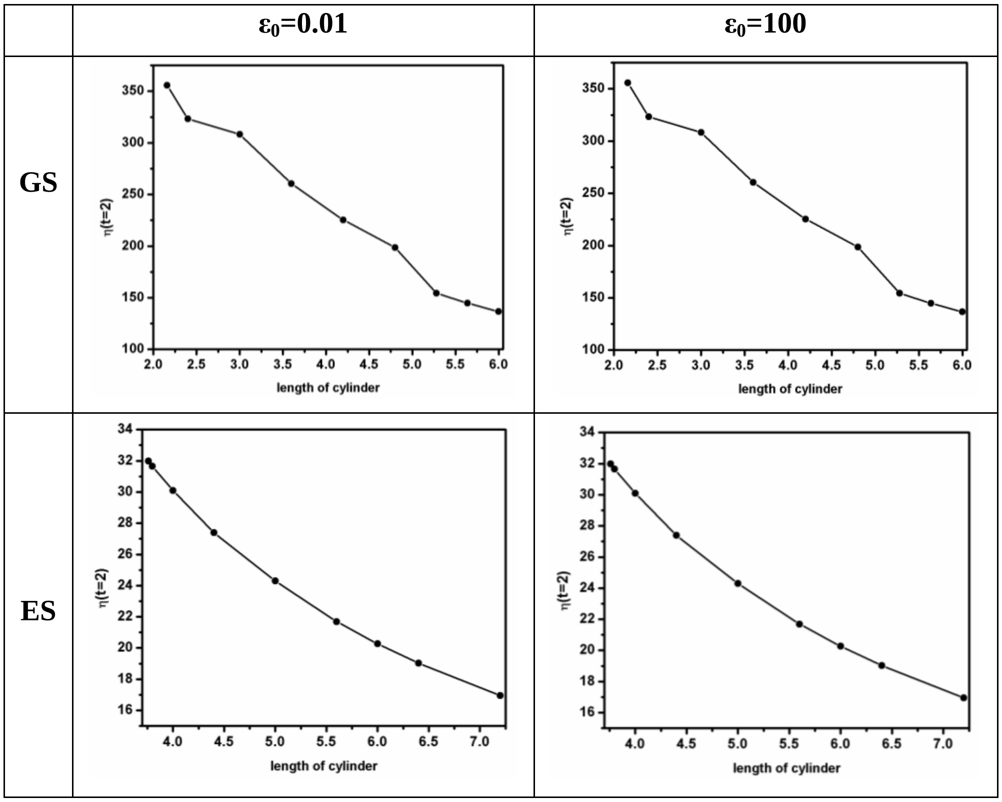


Figure S5: Plot of η(t = 2) vs. length of cylinder when N_2 molecule in GS and in first ES is placed in an external field ($\varepsilon_0 = 0.01$a.u. & 100a.u. and $\omega_0 = \pi$).

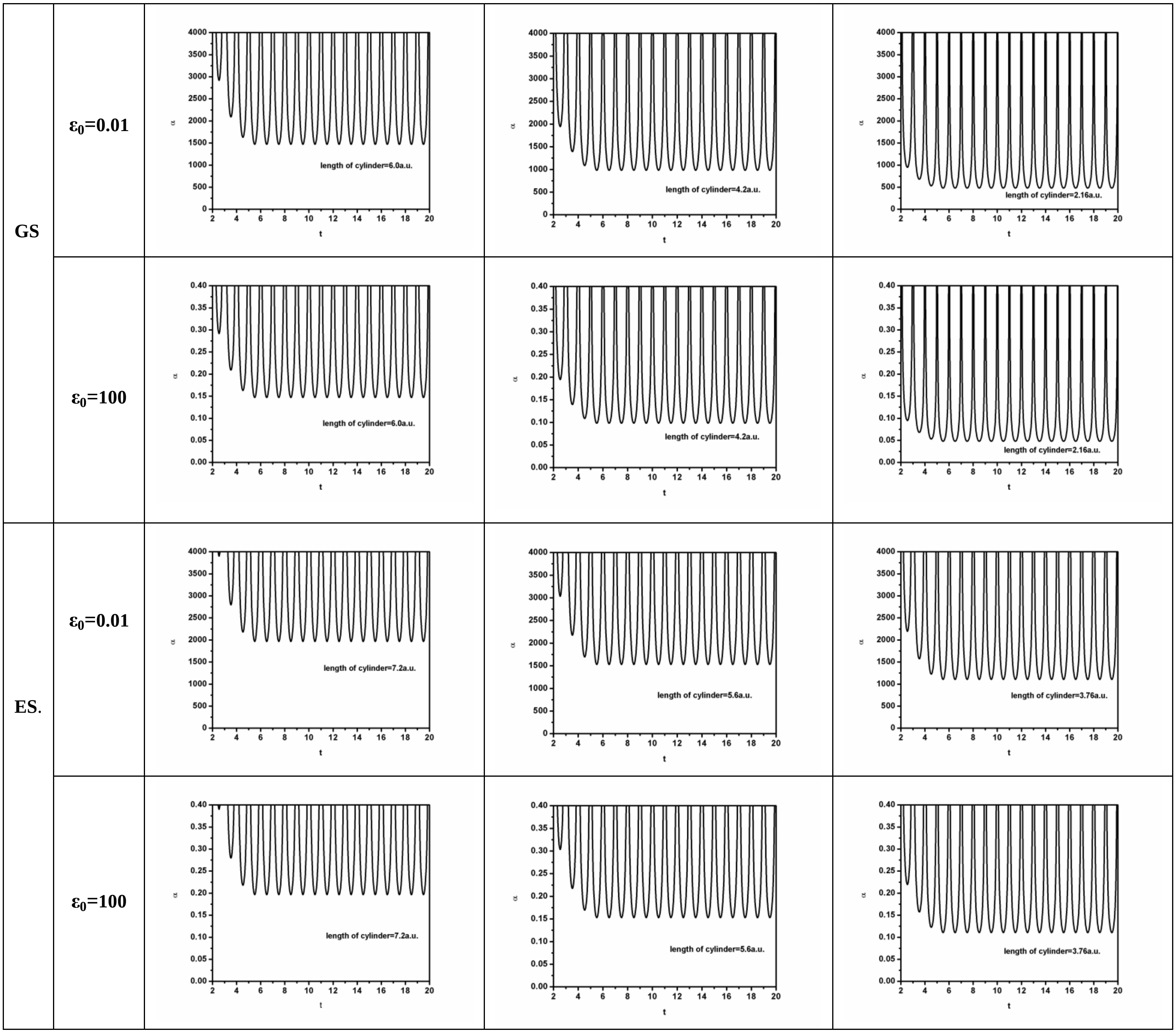


Figure S6: Time evolution of polarizability (α) when N_2 molecule in ground state (GS) and first excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

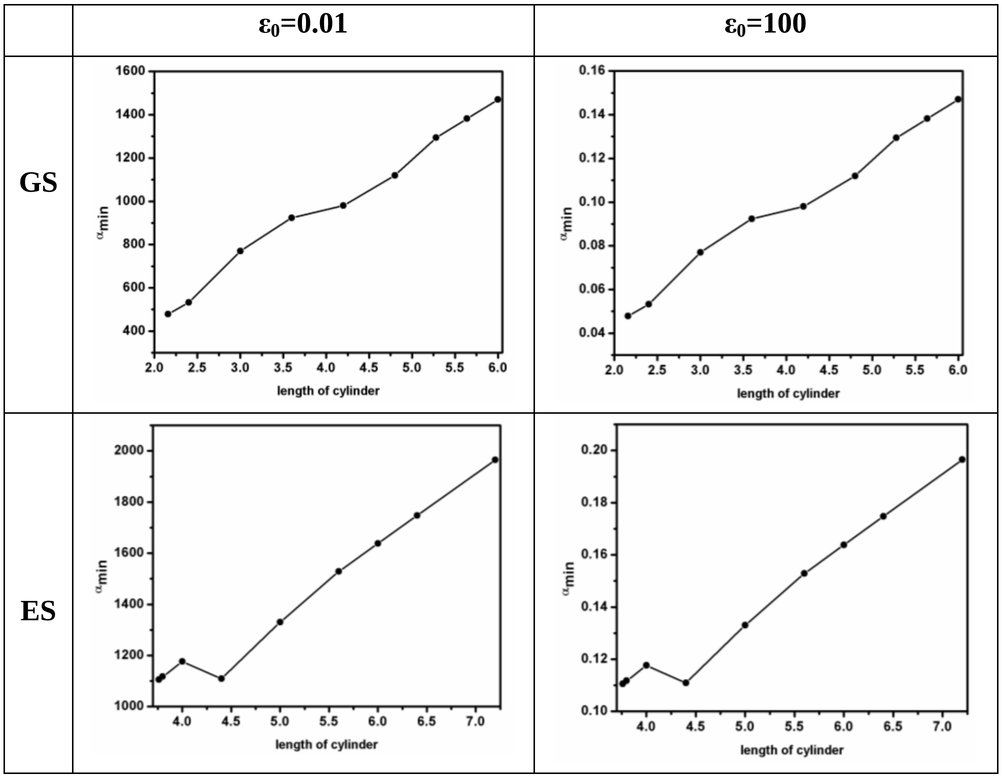


Figure S7: Plot of α_{min} vs. length of cylinder when N_2 molecule in GS and in first ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).

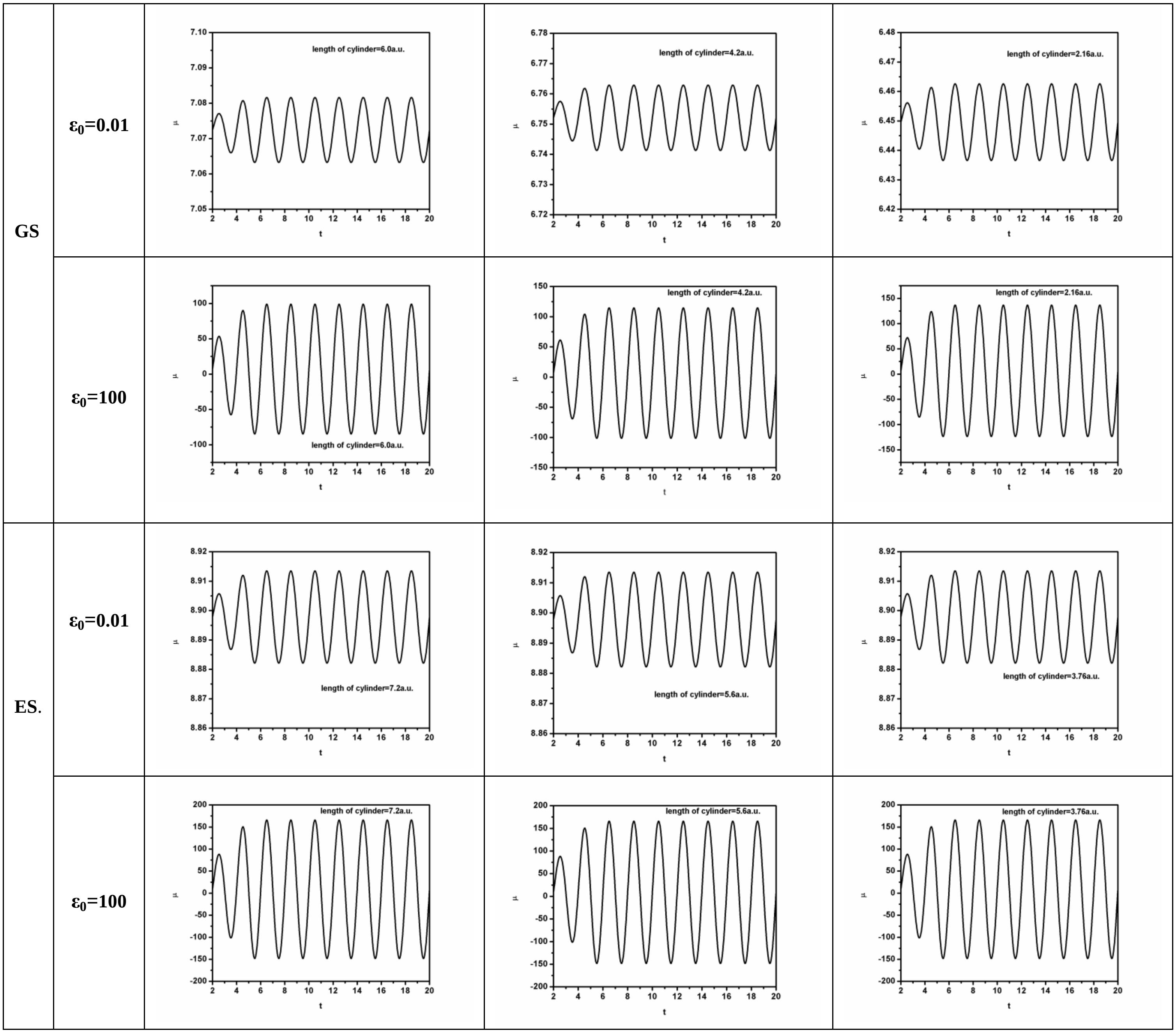


Figure S8: Time evolution of chemical potential (μ) when N_2 molecule in ground state (GS) and first excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

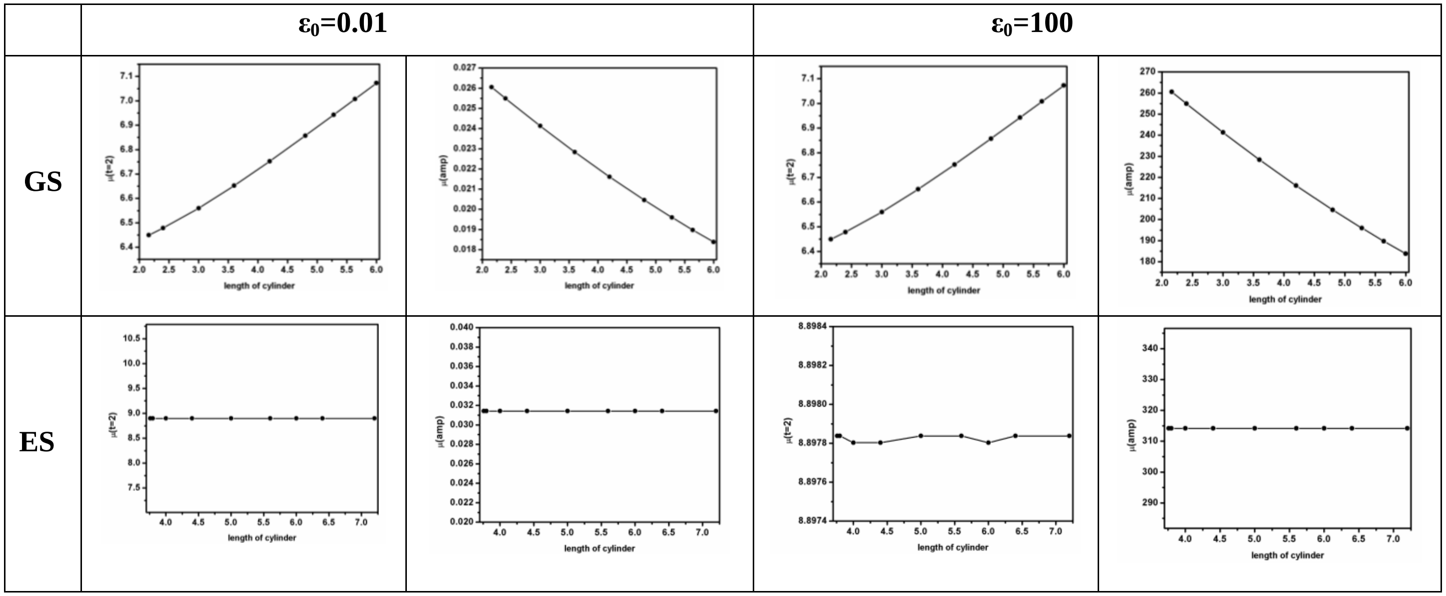


Figure S9: Plot of μ(t = 2) vs. length of cylinder and μ(amp) vs. length of cylinder when N_2 molecule in GS and in first ES is placed in an external field ($\varepsilon_0 = 0.01$a.u. & 100a.u. and $\omega_0 = \pi$).

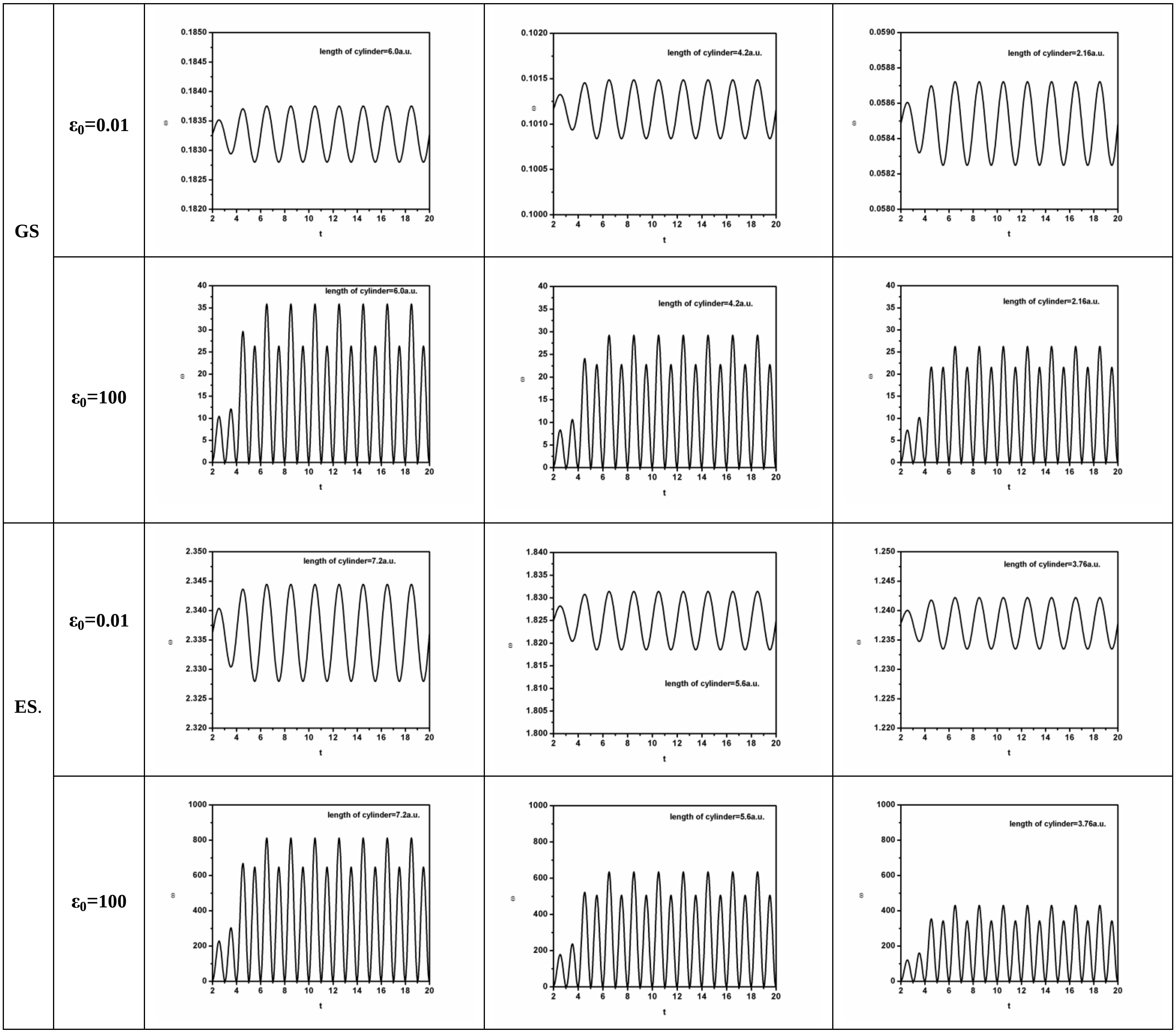


Figure S10: Time evolution of electrophilicity index (ω) when N_2 molecule in ground state (GS) and first excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

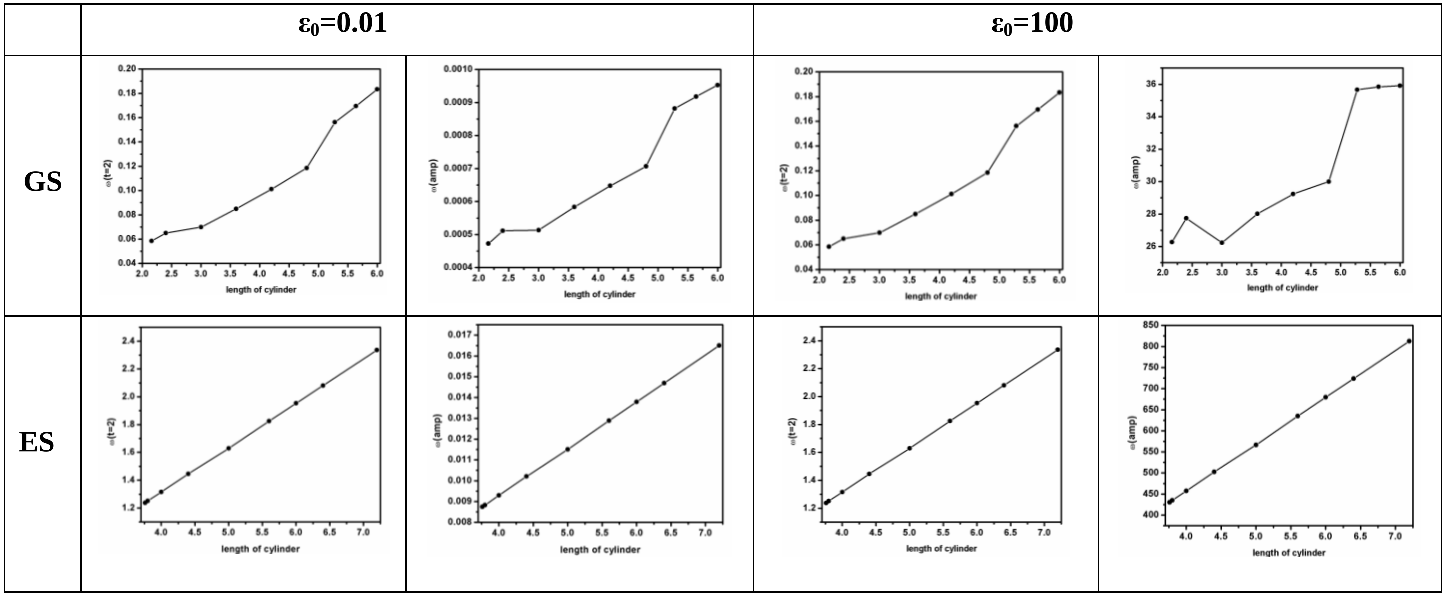


Figure S11: Plot of ω(t = 2) vs. length of cylinder and ω(amp) vs. length of cylinder when N_2 molecule in GS and in first ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).

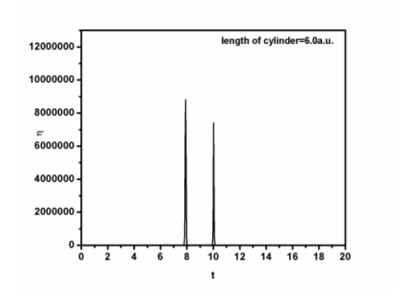
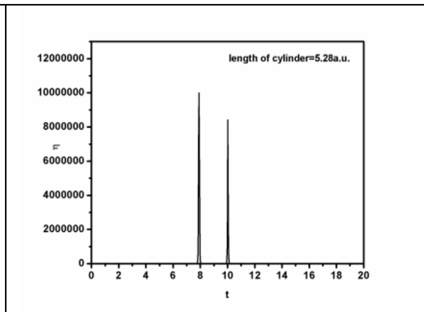
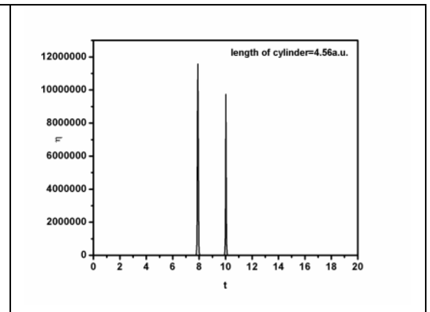
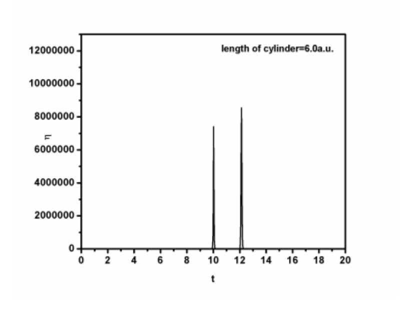
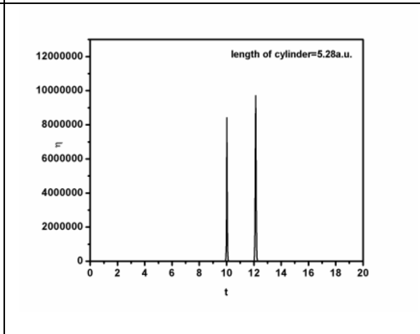
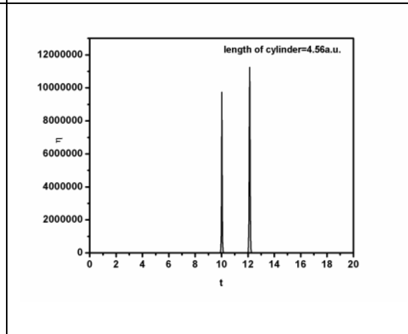
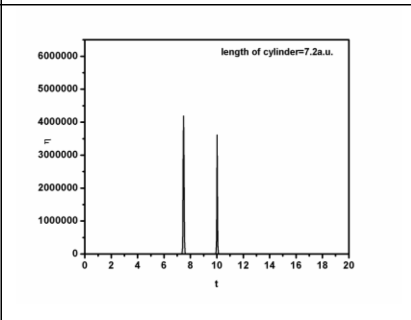
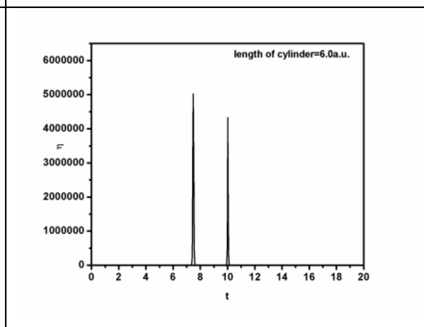
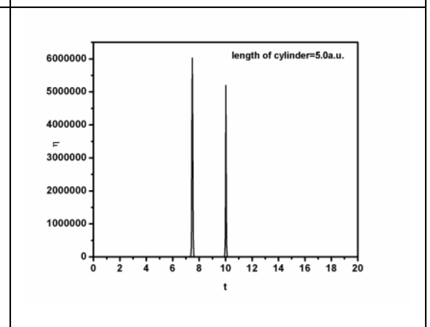
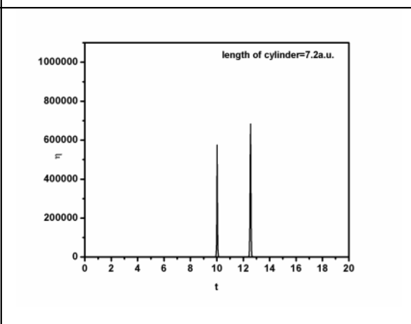
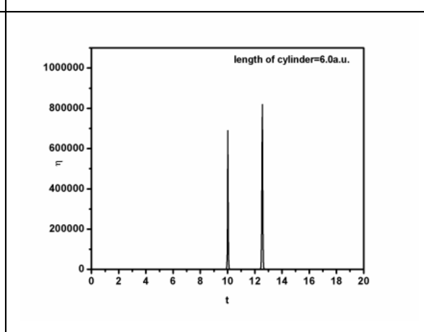
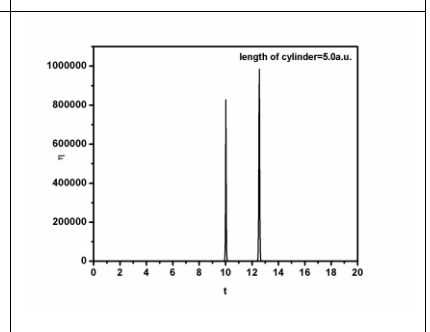
GS	**O side attack**			
	C side attack			
ES.	**O side attack**			
	C side attack			

Figure S12: Time evolution of chemical hardness (η) during a collision process between H^+ and CO molecule in ground state (GS) and excited state (ES) in a confined environment (length of cylinder = 6.0a.u. denotes unconfined system in GS and 7.2a.u. in ES).

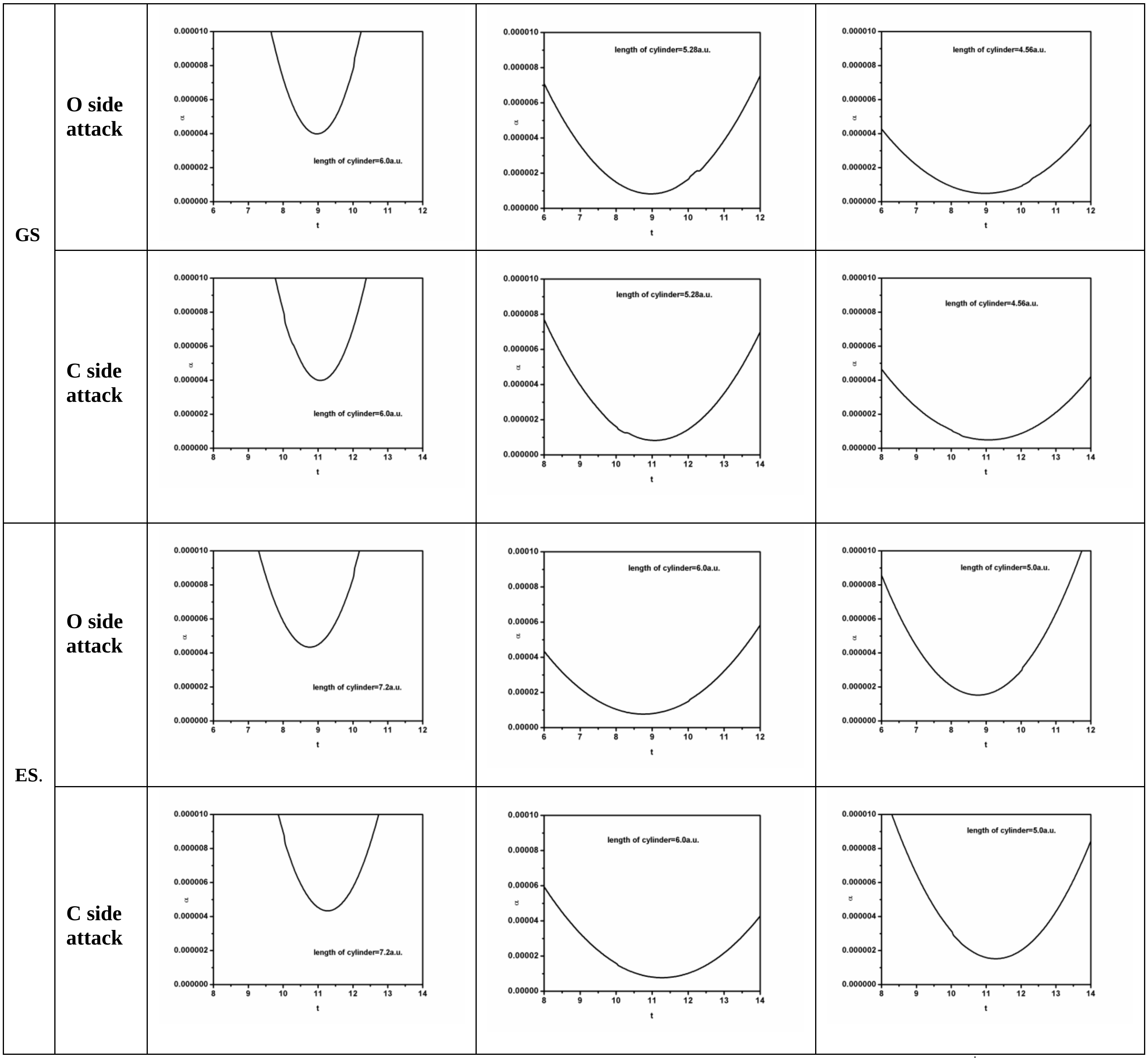


Figure S13: Time evolution of polarizability (α) during a collision process between H^+ and CO molecule in ground state (GS) and excited state (ES) in a confined environment (length of cylinder = 6.0a.u. denotes unconfined system in GS and 7.2a.u. in ES).

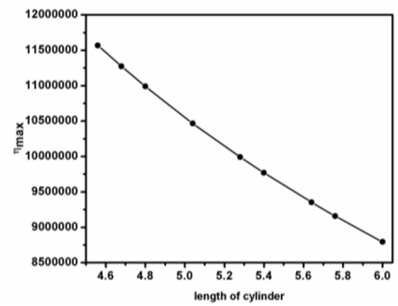
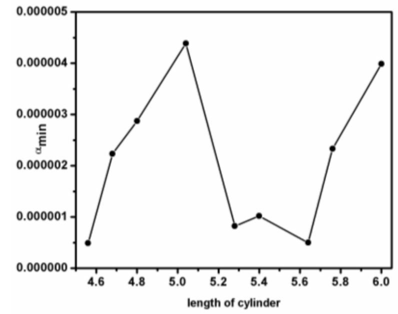
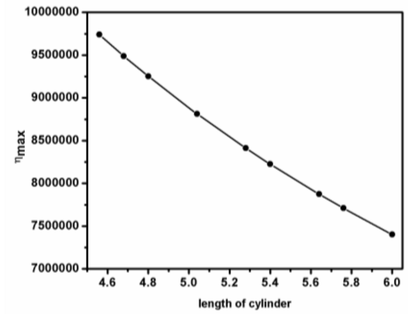
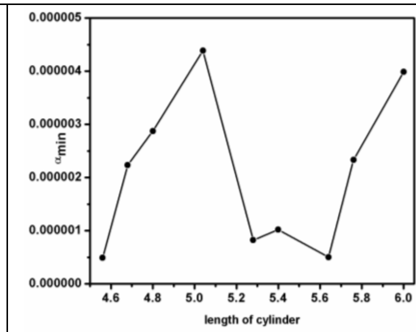
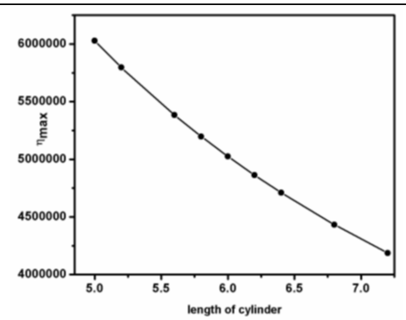
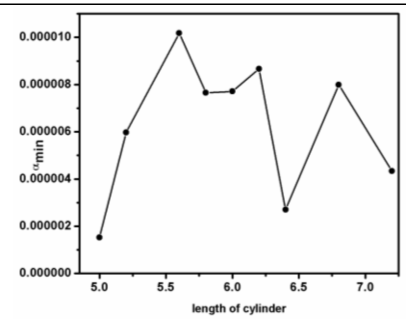
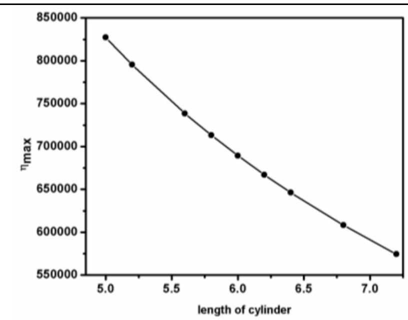
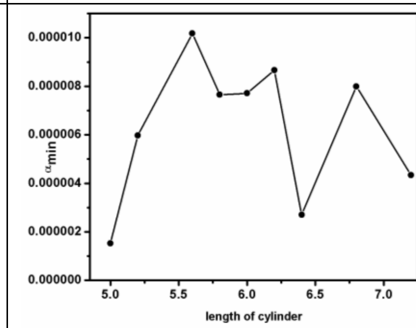
	O side attack		C side attack	
GS				
ES				

Figure S14: Plots of η_{max} vs. length of cylinder and α_{min} vs. length of cylinder during a collision process between H^+ and CO molecule in GS and ES.

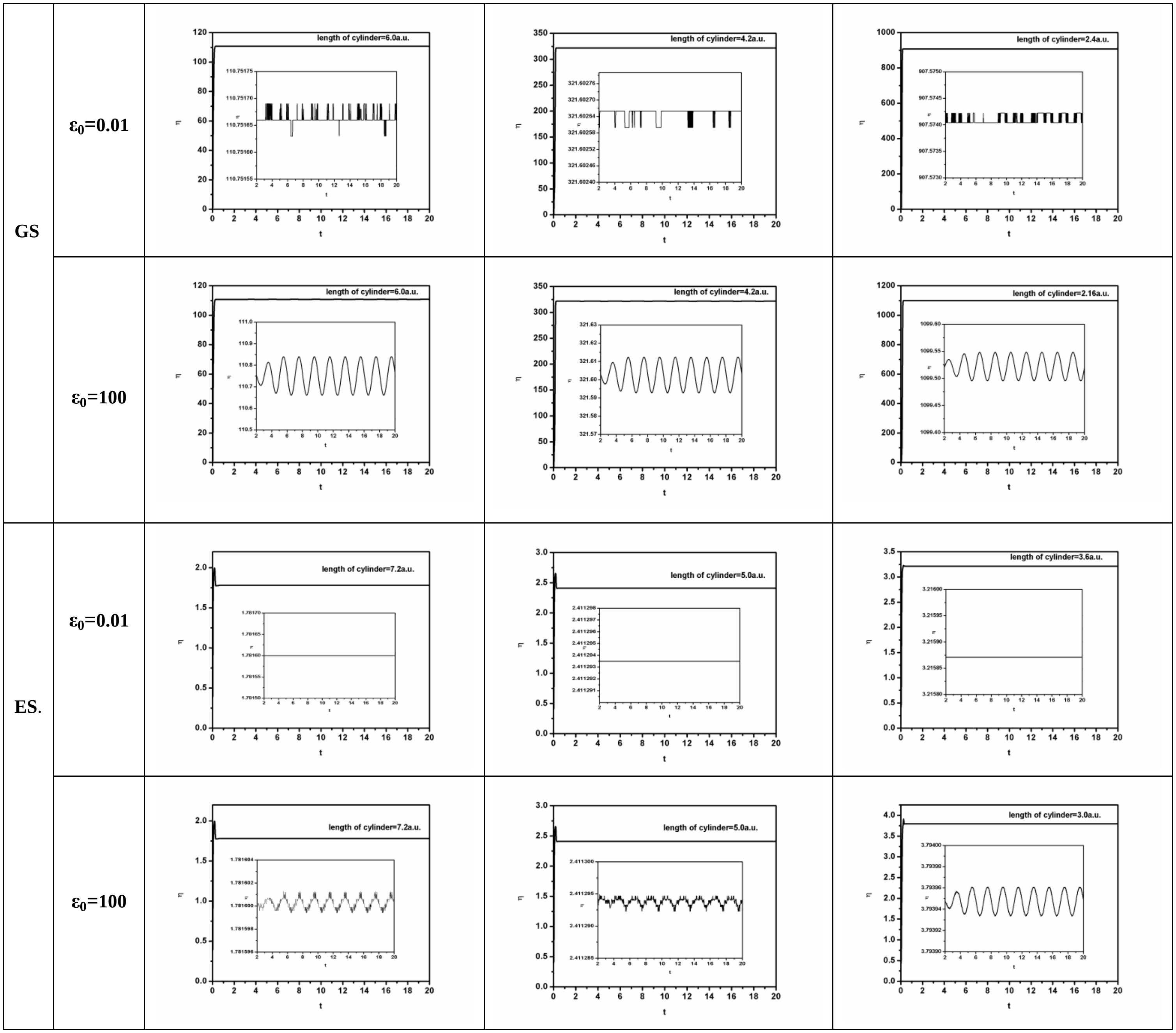


Figure S15: Time evolution of chemical hardness (η) when CO molecule in ground state (GS) and excited state (ES) is placed in an external field of amplitude $\varepsilon_0 = 0.01$a.u. & 100a.u. and frequency $\omega_0 = \pi$.

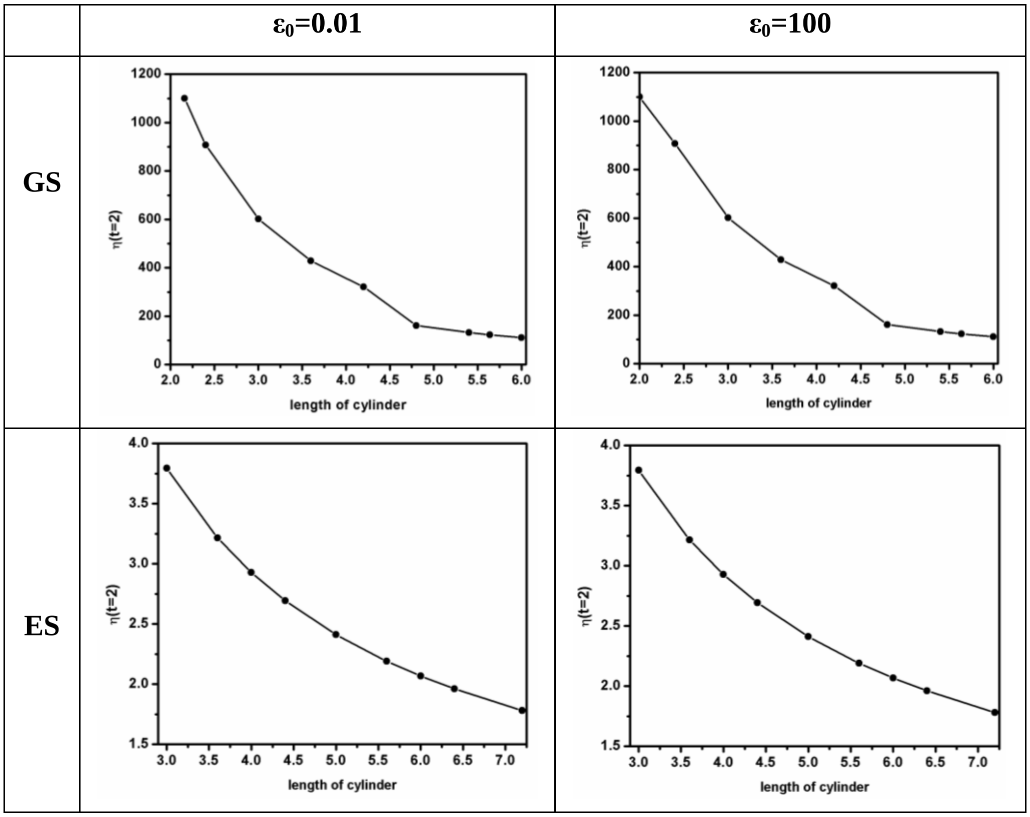


Figure S16: Plot of η(t = 2) vs. length of cylinder when CO molecule in GS and ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

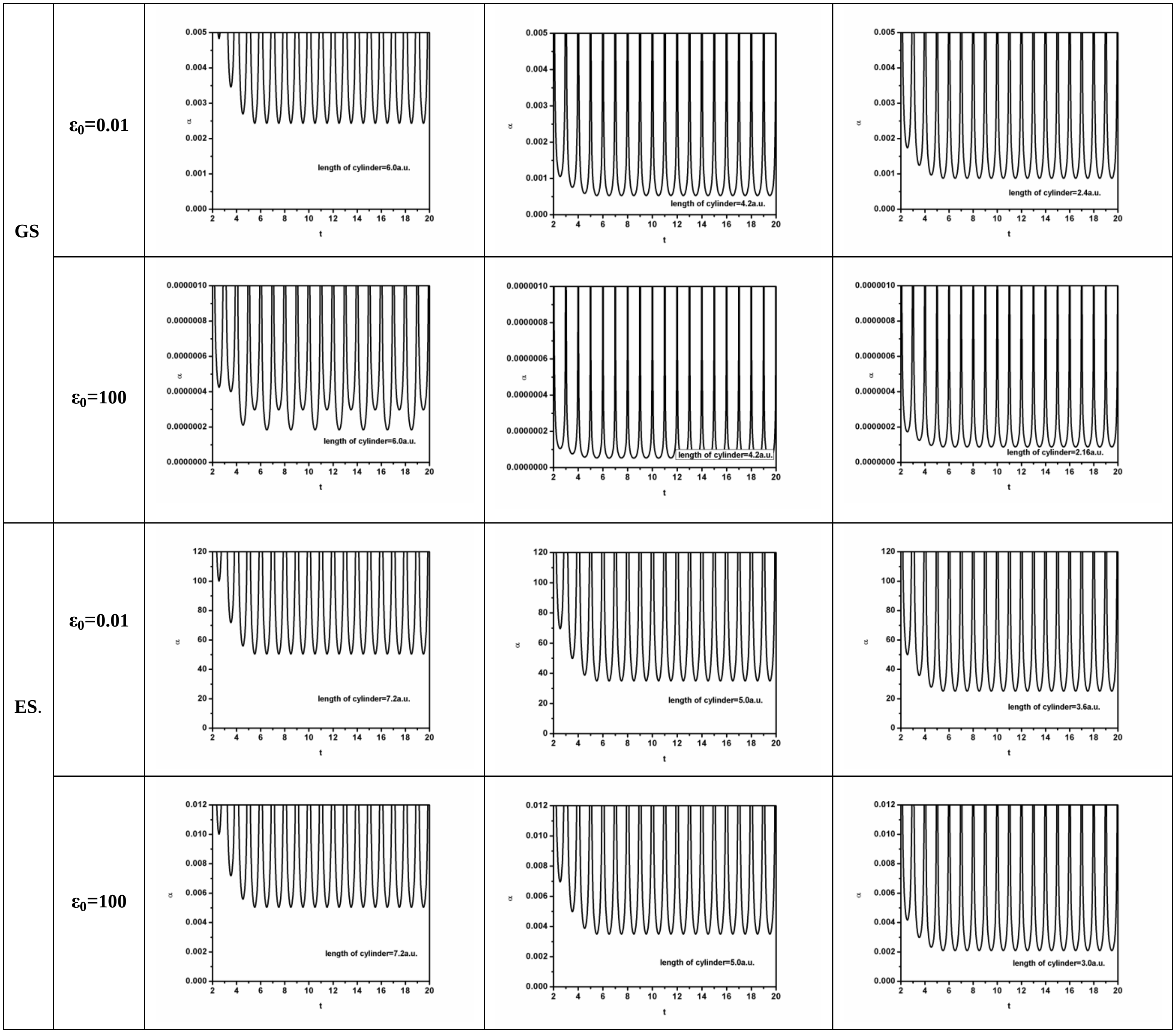


Figure S17: Time evolution of polarizability (α) when CO molecule in ground state (GS) and excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

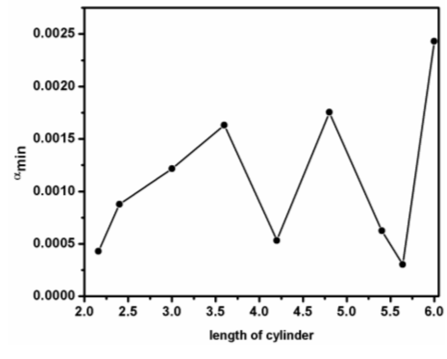
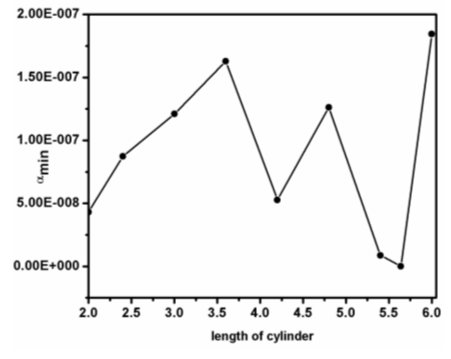
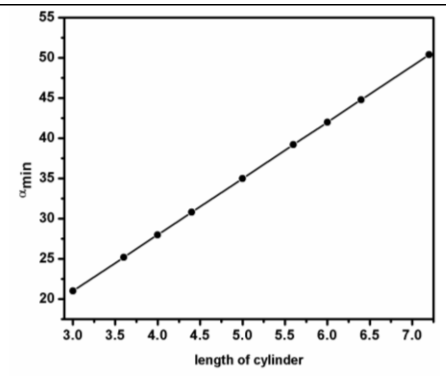
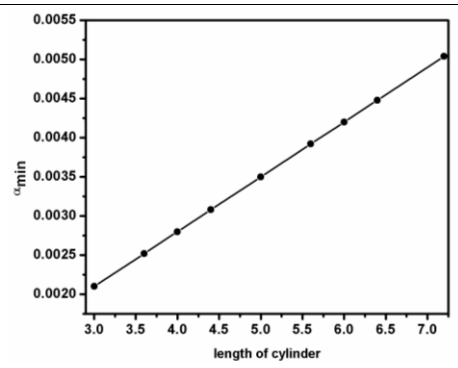
	ε_0=0.01	ε_0=100
GS		
ES		

Figure S18: Plot of α_{min} vs. length of cylinder when CO molecule in GS and ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).

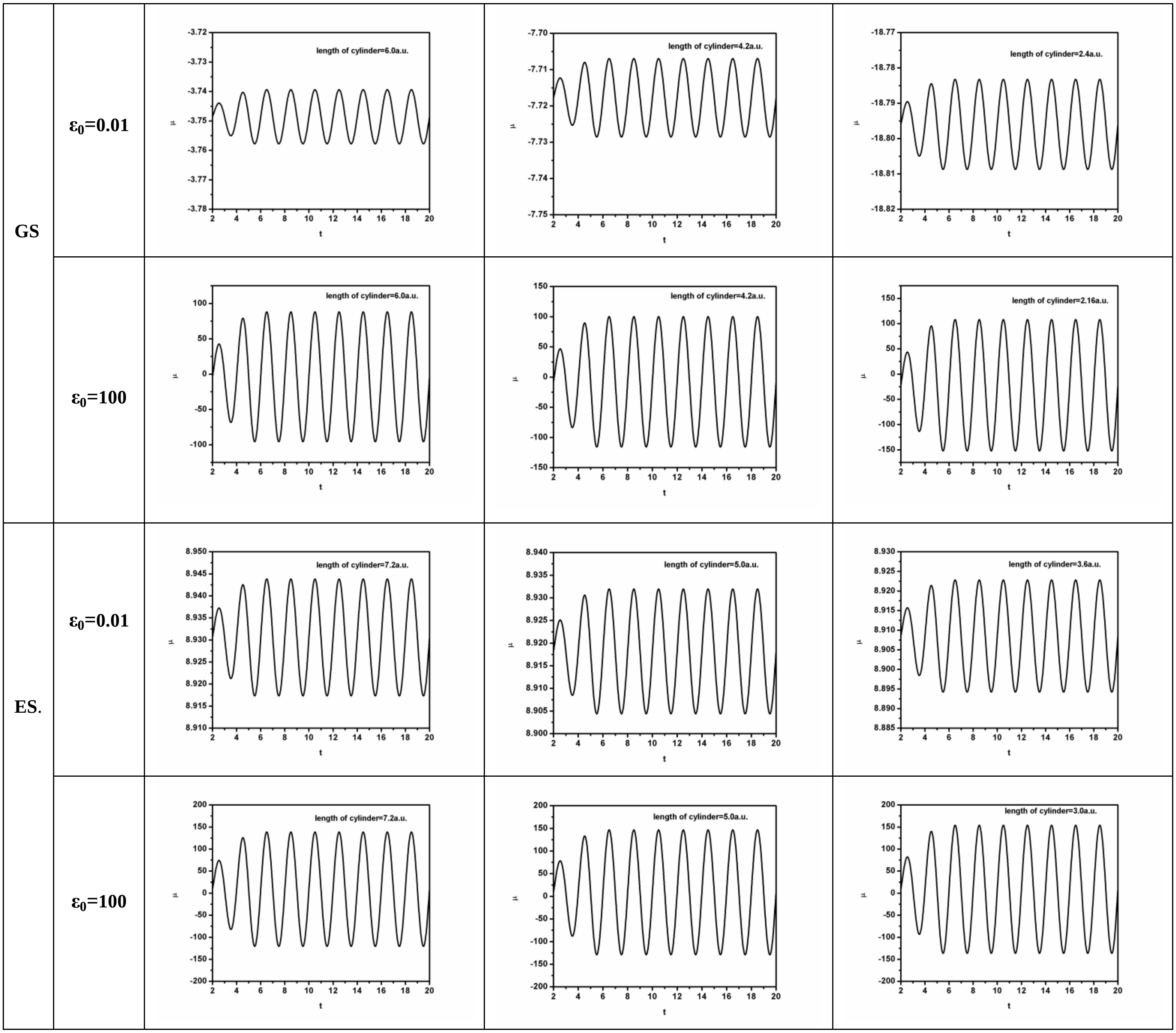


Figure S19: Time evolution of chemical potential (μ) when CO molecule in ground state (GS) and excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

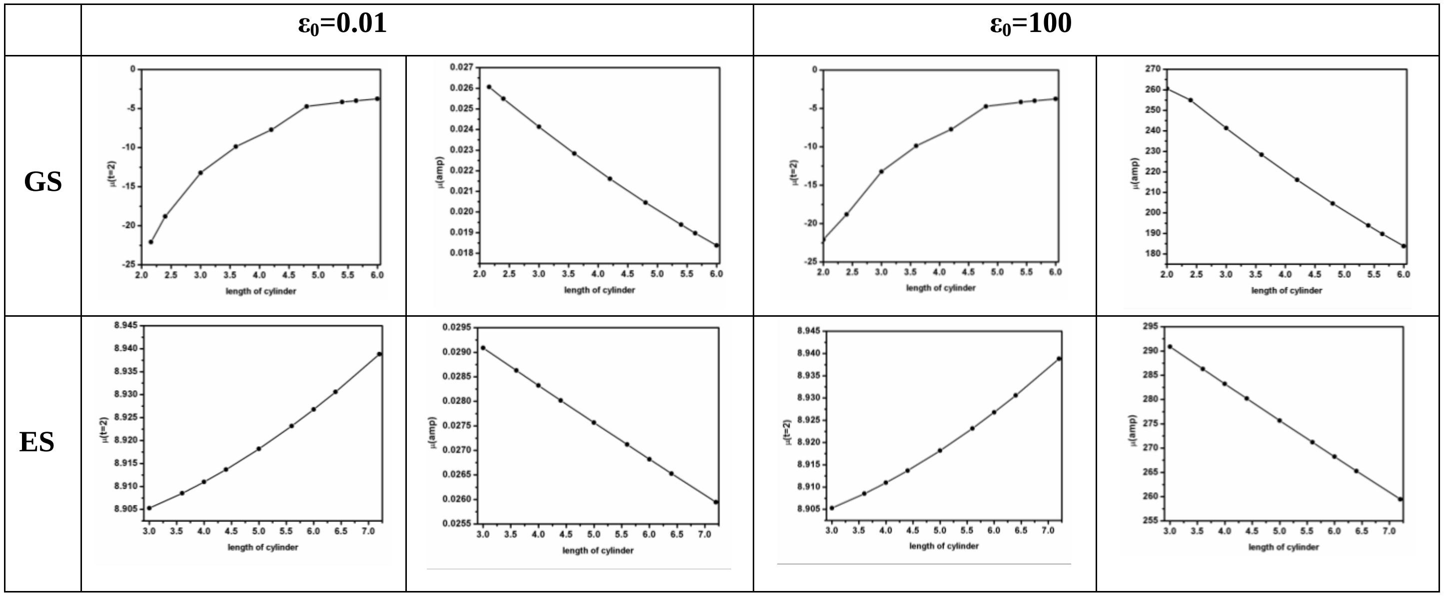


Figure S20: Plot of μ(t = 2) vs. length of cylinder and μ(amp) vs. length of cylinder when CO molecule in GS and ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).

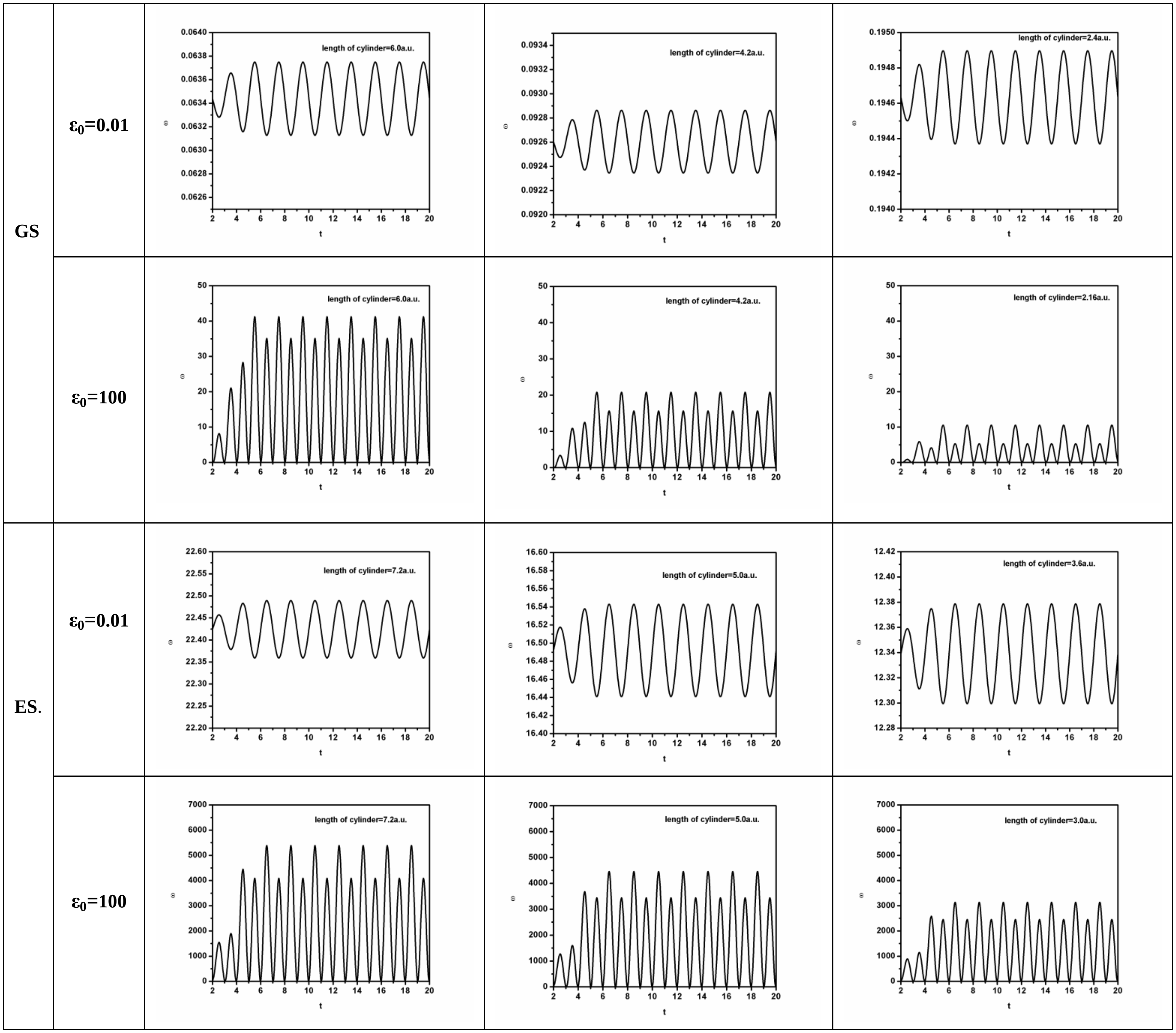


Figure S21: Time evolution of electrophilicity index (ω) when CO molecule in ground state (GS) and excited state (ES) is placed in an external field of amplitude ε_0 = 0.01a.u. & 100a.u. and frequency $\omega_0 = \pi$.

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

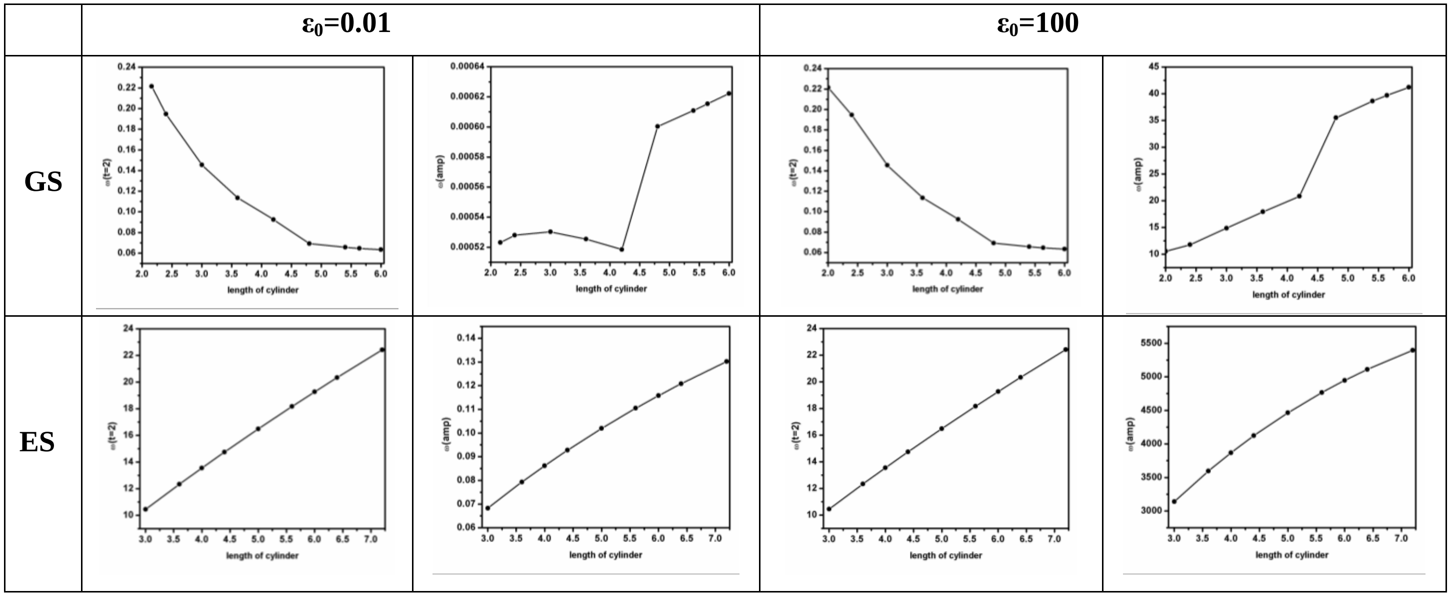


Figure S22: Plot of ω(t = 2) vs. length of cylinder and ω(amp) vs. length of cylinder when CO molecule in GS and ES is placed in an external field (ε_0 = 0.01a.u. & 100a.u. and $\omega_0 = \pi$).