Supporting Information

Stability of Molecular Layer Deposited Zincone films: Experimental and Theoretical exploration

Devika Choudhury,[a] Gopalan Rajaraman[b], Shaibal K. Sarkar[a]*

[a]Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai-400076, India.

[b]Department of Chemistry, Indian Institute of Technology Bombay, Mumbai-400076, India.

* Email id: shaibal.sarkar@iitb.ac.in

Tel: +9122 2576 7846;

Fax: +9122 2576 4890

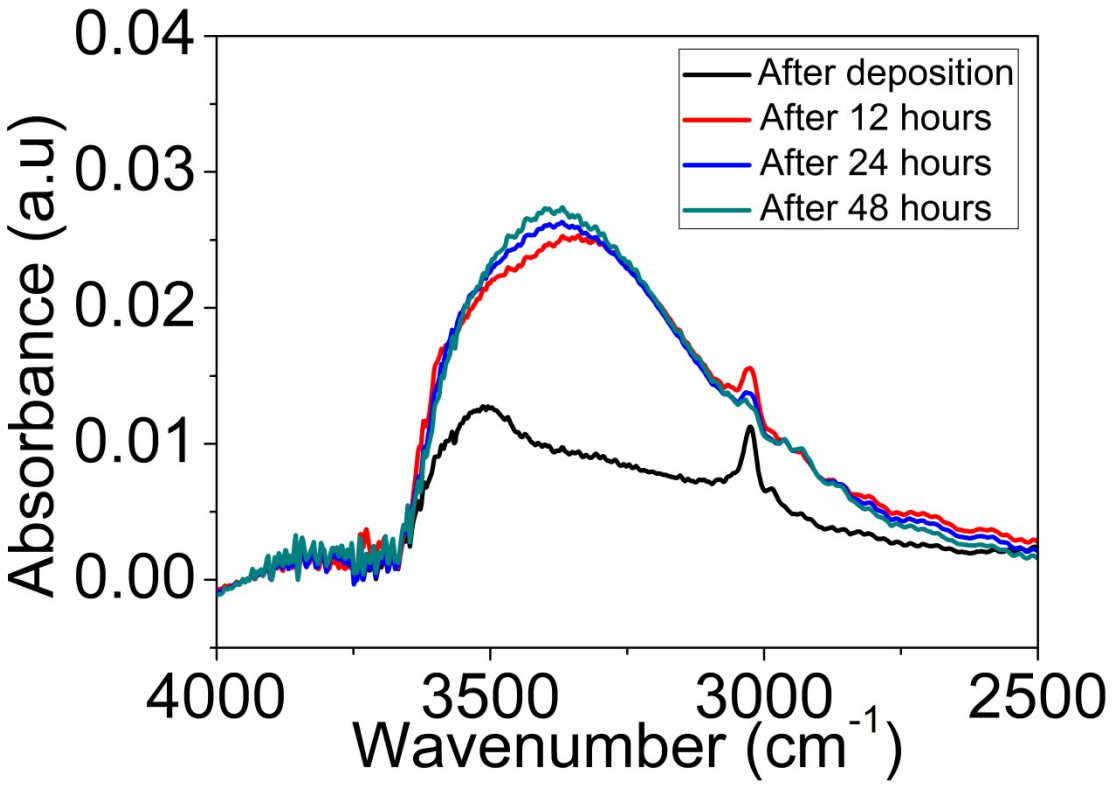

Figure SI-1. Increasing –OH vibration stretch observed in FTIR spectra of 300 cycles of Zincone film grown on KBr pallets and recorded over a time span of 48 hours.

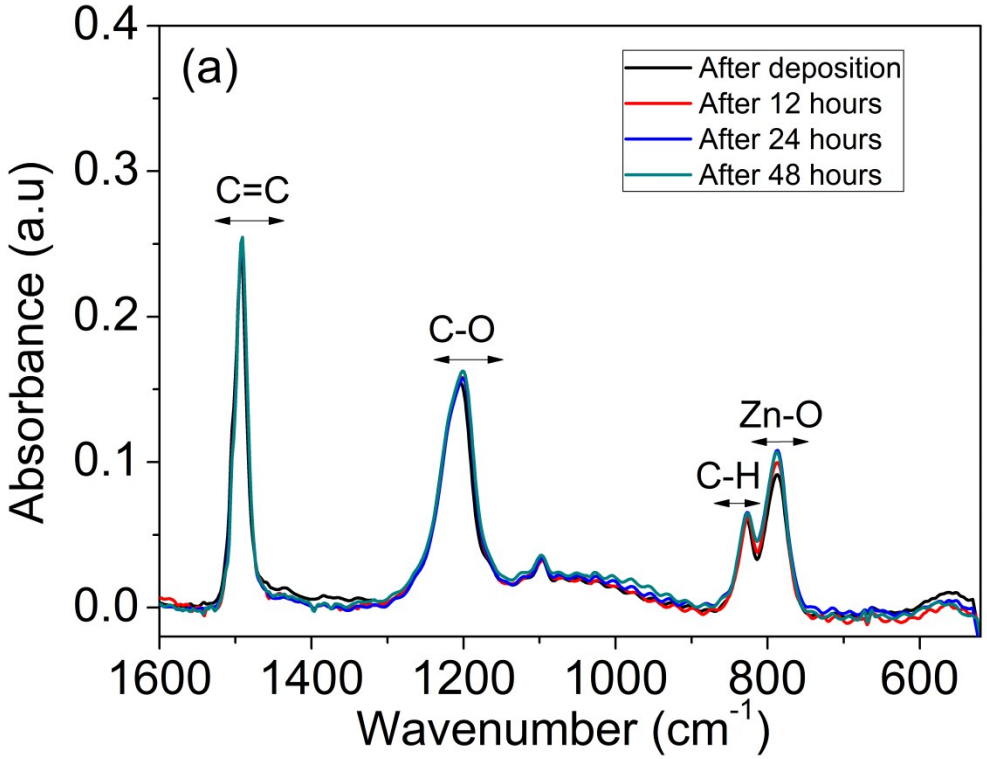

Figure SI-2. FTIR spectra of 300 cycles of Zincone film grown on KBr pallets and recorded over a time span of 48 hours. The sample under observation was in vacuum between each scan.

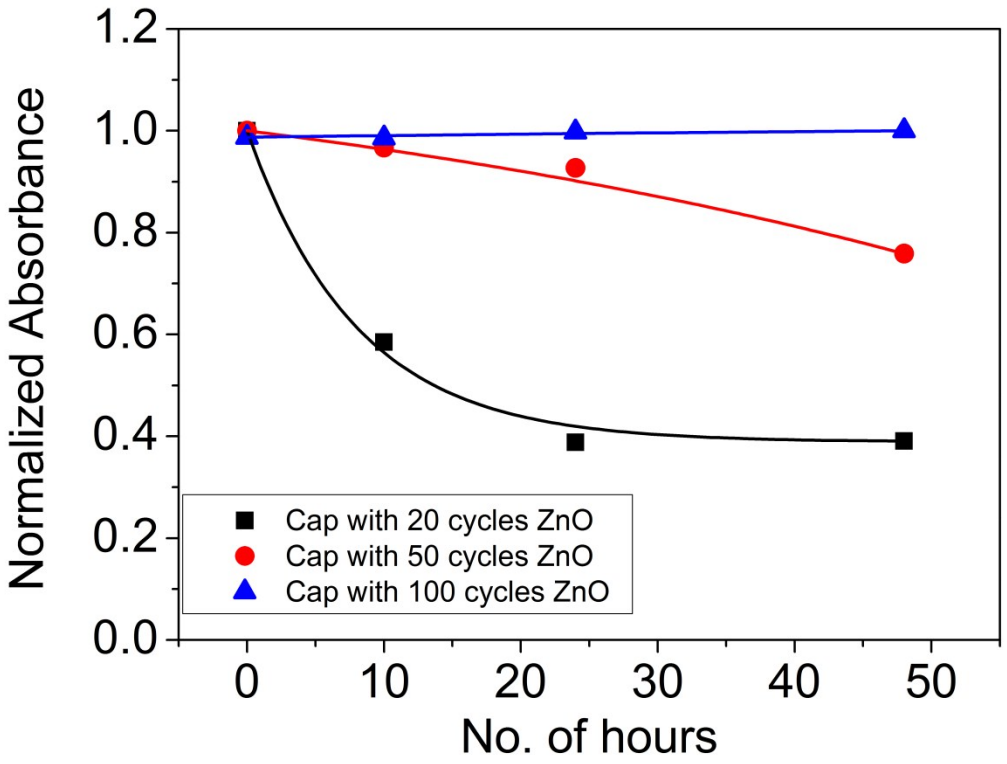

Figure SI-3. Variation in the absorbance intensity of Zn-O stretch (at 788cm^{-1}) with time with different ZnO capping thickness on it. With 100 cycles i.e ca. 20nm of ZnO capping prevents degradation of the Zn-O stretch and hence zincone material completely under ambient atmospheric conditions.

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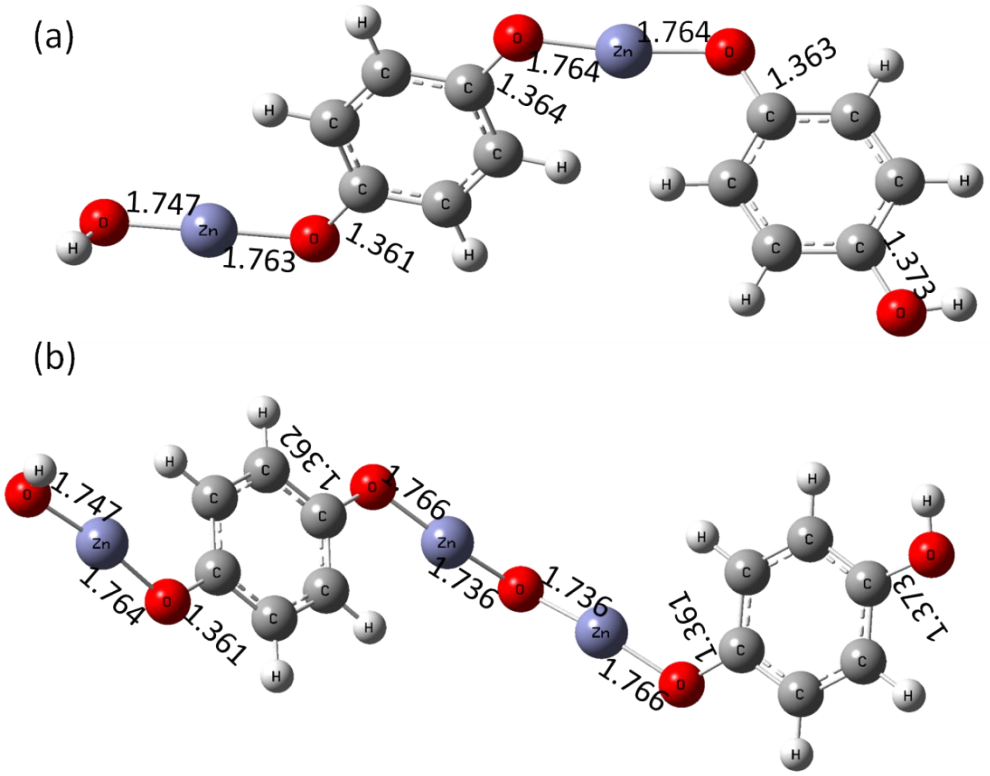

Figure SI-4. Bond lengths of (a) Two zincone molecules (b) Two zincone molecules with one ZnO moiety inserted in between as obtained from theoretical DFT calculations.

Description	Frequency of HQ (cm^{-1}) (reported)	Frequency of HQ (cm^{-1}) (Experimental)	Frequency of zincone after degradation (cm^{-1})
υ(CC)	1521	1518	1514
υ(CC)	1455	1471	1473
γ(CC)	1332	1352	1367
υ(CO)	1249	1241	1241
α(CH)	1178	1206	1216
α(CH)	1087	1095	1098
γ(CH)	821	828	827
β(CC)	754	759	757
δ(CO)	around 400	516	520

Table SI-1 Comparison of the different peak positions of various bond vibration stretches of zincone film after exposed to ambient for five days and only hydroquinone.

Reaction		Step	ΔE (KJ/mol
Reactant	Product		
$H_2O + Zn(C_2H_5)_2$	$[(HO)ZnC_2H_5]+ C_2H_6$	I	-120.2
$[(HO)ZnC_2H_5]$ + [(HO)Phenyl(OH)]	$[(HO)Zn(OPhenylOH)] + C_2H_6$	II	-84.7
[(HO)Zn(OPhenylOH)] + $Zn(C_2H_5)_2$	$[((HO)Zn(OPhenyl))OZnC_2H_5] + C_2H_6$	III	-127.1
$[(HO)Zn(OPhenyl)OZnC_2H_5]$ + [(HO)Phenyl(OH)]	$[(HO)(ZnOPhenylO)_2H)] + C_2H_6$	IV	-78.3
$[((HO)ZnOPhenyl)OZnC_2H_5]$ + H_2O	[((HO)ZnOPhenyl)OZn(OH)] + C_2H_6	V	-77.7
[((HO)ZnOPhenyl)OZn(OH)] + $Zn(C_2H_5)_2$	$[((HO)ZnOPhenylO)ZnOZnC_2H_5]$ + C_2H_6	VI	-132.8
$[((HO)ZnOPhenylO)ZnOZnC_2H_5]$ + [(HO)Phenyl(OH)]	$[((HO)ZnOPhenylO)_2ZnOH] + C_2H_6$	VII	-86.6
$[((HO)ZnOPhenylO)ZnOZnC_2H_5]$ + H_2O	$[((HO)ZnOPhenylO)ZnOZnOH]+ C_2H_6$	VIII	-82.8
[((HO)ZnOPhenylO)ZnOZnOH] + $Zn(C_2H_5)_2$	$[((HO)ZnOPhenylO)ZnOZnOZn C_2H_5]$ + C_2H_6	IX	-129.4
[((HO)ZnOPhenylO)ZnOZnOZn C_2H_5] + [(HO)Phenyl(OH)]	[((HO)ZnOPhenylO)ZnOZnOZnOPhenyl (OH)] + C_2H_6	X	-78.6

Table SI-2 Various reaction energies for different half surface reactions of zincone and zincone alloys.