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Study Interaction between Tin Dioxide Nanowhiskers and Ethanol Molecules in Gas Phase: Monte Carlo (MC) and Langevin Dynamics (LD) Simulation

L. Mahdavian, and M. Raouf

Abstract**—**Three dimensional nanostructure materials have attracted the attention of many researches because the possibility to apply them for near future devices in sensors, catalysis and energy related.

Tin dioxide is the most used material for gas sensing because its three-dimensional nanostructures and properties are related to the large surface exposed to gas adsorption. We propose the use of branch SnO_2 nanowhiskers in interaction with ethanol. All Sn atoms are symmetric. The total energy, potential energy and Kinetic energy calculated for interaction between SnO_2 and ethanol in different distances and temperatures. The calculations achieved by methods of Langevin Dynamic and Mont Carlo simulation. The total energy increased with addition ethanol molecules and temperature so interactions between them are endothermic.

Keywords**—**Tin dioxide, nanowhisker, Ethanol, Langevin Dynamic and Mont Carlo Simulation.

I. Introduction

IT has been suggested that nanometer sized particles, properly prepared and treated, might be used to form the high surface area analogues of known catalysts or sensors to provide improved efficiency of existing catalytic or sensor function [1], [2]. This might further be improved through changes in molecular electronic structure and as a result the development of confined regions that accompany the transition to the macroscopic regime for both the active elements and their substrate supports[3]. In this paper, we used tin dioxide because present great potential properties for applications as optoelectronic devices, gas sensor, solar energy or even for detecting leakages of reducing gases such as H, H_2S, CO and other[4]. Solids with a grain size of a few nanometers are normally referred to as nano[crystalline materials: they exhibit properties that are significantly different from their coarse-grained polycrystalline counterparts. A first classification of the change to the properties of a material relies on either "bulk" or "surface" effects.

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Typically bulk effects involve the confinement of electrons in nano-metric cells, which cause quantum phenomena to take place; an emblematic example is the dramatic change of optical properties of nano[structured silicon[5]. Surface effects normally appear because of the magnification in the specific surface of nanostructures, leading to the enhancement of the properties related to that, such as catalytic activity or surface adsorption [6].

Developing new solid-state gas sensors with improved properties carries with it an obvious close relationship between the sensing performance of the active materials and their surface chemical activity. The theoretical study of such surface adsorb interactions provides a valuable tool to get superior performances that are unattainable using only a trial-and-error approach together with a powerful analytic methodology to explain the experimental data. Tin dioxide (SnO_2) plays a key role as one of the more representative sensing materials in solid state gas sensors[7], presenting a significant surface reactivity with many important reducing (CO, NO) and oxidizing gases (O_2, NO_2) [8], [9]. However, to explain the sensing behavior it is necessary to keep in mind that there exists interfering processes poisoning the surface [10] and that these can dramatically change the effective adsorptions of the target species and, therefore, their eventual detection. In the case of the SnO_2 surface, SO_2 is one of the more relevant poison specimens [11], [12].

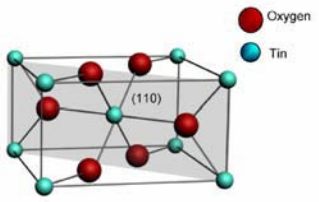

Fig. 1 Optimized configuration Top-view of Tin dioxide (SnO_2)

Thus, in the present analysis, its effects have also been studied in order to point up the consequences of the poisoning process on the sensing mechanisms[13].

In this paper, we used to branch SnO_2 nanowhiskers in a controlled approach of symmetric that shown in Fig. 1. After structural characterizations, photoluminescence characteristics of the branched SnO_2 nanowhiskers were studied. These branched SnO_2 nanowhiskers should find many promising interactions with ethanol in gas phase, that three-dimensional optoelectronic devices and gas sensors applications.

Nowadays, first-principles methodologies based on Langevin Dynamic simulation and Mont Carlo simulation can provide precise calculations of the total energetic and potential energy of the adsorption. Moreover, faster codes and new computational facilities allow dealing with numbers of surface adsorb configurations in moderate computing times. In this context, the aim of the present work is to provide theoretical hints for the development of improved C_2H_5OH gas sensors using SnO_2 as the base sensing material that a pattern interaction between SnO_2 nanowhiskers and 50 molecules ethanol in mean distance 16.54 A^o shown in Fig. 2. The surface orientation relevance is discussed, and the most significant adsorption sites of C_2H_5OH are identified.

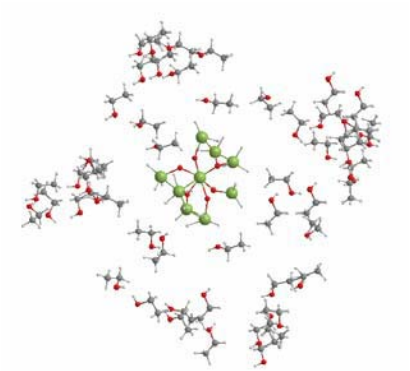

Fig. 2 Interaction between SnO_2 nanowhiskers and ethanol molecules in mean distance 16.52 A^o

II. Calculation Details

A. Langevin Dynamics (LD) Simulation

The Langevin equation is a *stochastic* differential equation in which two force terms have been added to Newton's second law to approximate the effects of neglected degrees of freedom.[14] One term represents a frictional force, the other a *random* force $\vec{R}$. For example, the effects of solvent molecules not explicitly present in the system being simulated would be approximated in terms of a frictional drag on the solute as well as random kicks associated with the thermal motions of the solvent molecules. Since friction opposes motion, the first additional force is proportional to the particle's velocity and oppositely directed. Langevin's equation for the motion of atom *i* is [15]:

$$\vec{F_i} - \gamma_i \vec{\upsilon}_i + \vec{R}_i(t) = m_i \vec{a}_i \qquad (1)$$

Where, $\vec{F_i}$ is still the sum of all forces exerted on atom *i* by other atoms explicitly present in this system. This equation is often expressed in terms of the `collision frequency $\zeta = \gamma / m$.

The friction coefficient is related to the fluctuations of the random force by the *fluctuation-dissipation theorem*:

$$\left\langle \vec{R}_i(t) \right\rangle = 0$$

$$\int \left\langle \vec{R}_i(0).\vec{R}_i(t) \right\rangle dt = 6K_B T \gamma_i \qquad (2)$$

In simulations it is often assumed that the random force is completely uncorrelated at different times. That is, the above equation takes the form:

$$\left\langle \vec{R}_i(t).\vec{R}_i(t') \right\rangle dt = 6K_B T \gamma_i \delta(t - t') \qquad (3)$$

The temperature of the system being simulated is maintained via this relationship between $\vec{R}(t)$ and γ. The jostling of a solute by solvent can expedite barrier crossing, and hence Langevin dynamics can search conformations better than Newtonian molecular dynamics ($\gamma = 0$).

B. Molecular Mechanics (Monte Carlo (MC) Simulation)

The Metropolis implementation of the Monte Carlo algorithm has been developed to study the equilibrium thermodynamics of many-body systems. Choosing small trial moves, the trajectories obtained applying this algorithm agree with those obtained by Langevin's dynamics [16]. To effectively search the resultant energy landscape, we exploit the recently developed parallel hyperbolic sampling algorithm in our Monte Carlo (MC) simulations. Previously, this protocol was shown to be more effective than general replica sampling in searching for low-energy structures, especially for proteins of large size where the energy landscape is significantly more rugged than the energy landscape of small proteins [17]. We introduce two quantities dependent on the cluster density and the combination of energy and free energy, which are more discriminative than the generally used average energy and cluster size for the identification of near-native structures. This is understandable because the Monte Carlo simulations always detect the so-called "important phase space" regions that are of low energy [18]. Because of imperfections of the force field, this lowest energy basin usually does not correspond to the native state in most cases, so the rank of native structure in those decoys produced by the force field itself is poor. Therefore, the rank of native structure can be relatively better when ranked by the second force field [19]. Molecular Mechanics (MM) is widely used to simulate many particle systems ranging from solids, liquids, gases, and bimolecular on Earth, to the motion of stars and galaxies in the Universe. Newton's equations of motion for the system are integrated numerically. If the system is in equilibrium, static properties such as temperature and pressure are measured as averages over time.

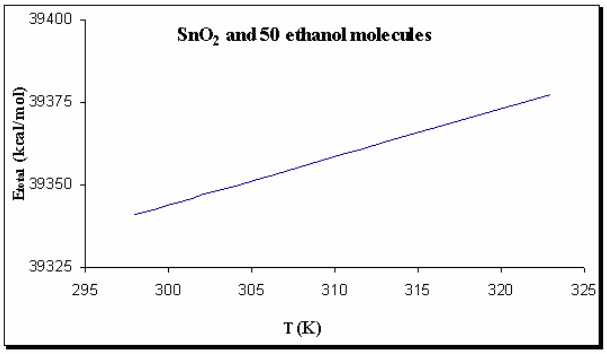

Fig. 3 The total energy (kcal/mol) calculated for interaction SnO_2 and ethanol in mean distance 6.31A^o and different temperatures by Langevin Dynamin simulation

III. Results

TABLE I
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANO-WHISKERS AND FIVE ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =5)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
6.77	429.58	1534.52	1964.11	430.88	1534.47	1965.36	432.63	1535.50	1968.13	442.15	1536.11	1971.54
8.72	478.41	1274.32	1752.77	479.58	1274.42	1753.99	481. 98	1274.60	1756.50	484.22	1274.79	1759.00
9.85	580.37	1368.04	1948.41	581.54	1368.18	1949.72	507.26	1265.36	1772.62	509.56	1265.77	1775.34
11.23	122.40	865.24	987.64	123.51	865.38	988.89	125.73	865.66	991.39	127.96	865.94	993.90
12.60	127.67	860.29	987.96	128.85	860.37	989.21	131.19	860.52	991.72	133.55	860.68	994.23
13.21	127.70	860.39	988.08	128.87	860.46	989.34	131.22	860.62	991.84	133.57	860.78	994.35
14.02	78.54	784.06	862.60	79.67	784.18	863.85	81.94	784.42	866.36	84.20	784.66	868.87
18.79	78.54	984.09	1062.63	79.67	984.21	1063.88	81.93	984.46	1066.39	84.20	984.70	1068.90

TABLE II
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANO-WHISKERS AND FIVE ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =5)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
6.77	75.36	1889.87	1965.23	76.63	1887.48	1964.11	79.15	1889.91	1969.06	81.68	1891.88	1973.56
8.72	75.36	1675.77	1751.13	76.63	1676.49	1753.12	79.15	1676.86	1756.01	81.68	1677.62	1759.30
9.85	75.36	1867.98	1943.34	76.63	1868.36	1944.99	79.15	1691.42	1770.57	81.68	1691.99	1773.67
11.23	75.36	917.30	992.66	76.63	917.32	993.95	79.15	917.63	996.78	81.68	917.85	999.53
12.60	75.36	916.35	991.71	76.63	916.35	992.98	79.15	916.53	995.68	81.68	916.72	998.40
13.21	75.36	916.16	991.52	76.63	916.16	992.79	79.15	916.35	995.50	81.68	916.62	998.30
14.02	75.36	794.55	869.91	76.63	794.56	871.19	79.15	795.04	874.19	81.68	795.03	876.71
18.79	75.36	794.57	869.93	76.63	794.58	871.21	79.15	795.12	874.27	81.68	795.13	876.81

TABLE III
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANO-WHISKERS AND TEN ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =10)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
5.56	573.40	3444.84	4018.24	575.19	3445.049	4020.23	578.71	3445.36	4024.08	582.24	3445.68	4027.92
7.10	185.70	1110.80	1296.49	221.73	1111.34	1333.06	225.50	1111.41	1336.91	229.28	1111.48	1340.76
8.32	216.92	977.61	1194.53	218.79	977.66	1196.45	222.54	977.76	1200.30	226.29	977.86	1204.15
9.50	175.34	867.85	1043.19	177.20	867.89	1045.09	180.95	867.99	1048.94	183.07	866.76	1049.82
10.98	172.08	876.41	1048.49	173.91	876.51	1050.42	177.57	876.70	1054.27	181.22	876.89	1058.12
11.80	172.00	882.45	1054.45	173.84	882.58	1056.43	177.50	882.78	1060.28	181.15	882.97	1064.13
12.30	115.85	807.70	923.56	117.59	807.87	925.47	121.09	808.23	929.32	124.58	808.59	933.17
14.40	163.57	1321.80	1485.37	165.31	1322.01	1487.32	168.81	1322.37	1491.17	172.30	1322.72	1495.02

TABLE IV
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANO-WHISKERS AND TEN ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =10)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
5.56	115.73	3913.26	4029.00	117.68	3913.76	4031.43	121.56	3916.58	4038.14	125.44	3917.66	4043.11
7.10	115.73	1215.86	1331.59	117.68	1215.97	1333.64	121.56	1216.09	1337.65	125.44	1216.14	1341.58
8.32	115.73	1085.40	1201.14	117.68	1085.40	1203.08	121.56	1085.43	1206.99	125.44	1085.45	1210.89
9.50	115.73	933.87	1049.60	117.68	933.85	1051.53	121.56	933.86	1055.42	125.44	929.74	1055.18
10.98	115.73	939.75	1055.49	117.68	939.937	1057.61	121.56	939.95	1061.50	125.44	940.10	1065.54
11.80	115.73	945.36	1061.09	117.68	945.55	1063.23	121.56	945.56	1067.12	125.44	945.56	1071.01
12.30	115.73	815.86	931.59	117.68	815.86	933.54	121.56	815.86	937.42	125.44	815.94	941.38
14.40	115.73	1381.60	1497.33	117.68	1381.72	1499.39	121.56	1381.76	1503.32	125.44	1382.00	1507.45

TABLE V
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANO-WHISKERS AND TWELVE ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =20)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}
5.95	3223.26	13107.44	16330.71	3226.42	13107.56	16333.97	3232.71	13107.79	16340.51	3239.01	13108.03	16347.04
6.44	2418.76	9858.25	12277.01	2422.13	9858.14	12280.28	2428.88	9857.93	12286.81	2435.60	9857.73	12293.34
7.55	873.08	2902.55	3775.06	876.05	2902.83	3778.89	882.03	2903.40	3785.42	888.02	2903.95	3791.96
8.32	718.65	2302.10	3020.75	721.74	2302.28	3024.02	727.93	2302.63	3030.56	734.11	2302.98	3037.09
9.00	295.94	1556.50	1852.43	299.00	1556.74	1855.75	305.13	1557.16	1862.21	311.24	155.76	186.88
10.20	501.39	1875.76	2377.14	504.56	1875.87	2380.43	510.90	1876.06	2386.96	517.24	1876.25	2393.50
11.81	205.80	837.16	1042.96	208.90	837.30	1046.20	208.90	837.30	1046.20	221.31	837.96	1059.27
13.73	609.01	2019.43	2628.44	612.03	2019.75	2631.77	618.02	2020.29	2638.31	624.02	2020.82	2644.85

TABLE VI
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANO-WHISKERS AND TWELVE ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =20)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}
5.95	196.48	16146.68	16343.16	199.78	16148.93	16348.70	206.37	16152.31	16358.68	213.00	16156.03	16369.00
6.44	196.48	12085.93	12282.40	199.78	12086.33	12286.10	206.37	12083.45	12289.82	213.00	12083.78	12296.74
7.55	196.48	3555.64	3752.12	199.78	3555.84	3755.61	206.37	3556.53	3762.89	213.00	3557.71	3770.67
8.32	196.48	2813.03	3009.51	199.78	2813.41	3013.18	206.37	2814.63	3021.00	213.00	2814.66	3027.63
9.00	196.48	1667.82	1864.30	199.78	1667.99	1867.77	206.37	1668.22	1874.58	213.00	1668.25	1881.21
10.20	196.48	2182.76	2379.23	199.78	2182.76	2382.54	206.37	2183.42	2389.78	213.00	2183.42	2396.38
11.81	196.48	855.70	1052.18	199.78	855.72	1055.50	206.37	855.96	1062.33	213.00	856.19	1069.15
13.73	196.48	2424.00	2620.48	199.78	2424.81	2624.59	206.37	2425.09	2631.46	213.00	2425.75	2638.71

TABLE VII
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANOWHISKERS AND THIRTY ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =30)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}
5.92	11256.88	23855.66	35112.55	11261.20	23856.00	35117.21	11269.82	23856.61	35126.43	11278.44	23857.21	35135.65
6.63	5901.14	14672.38	20573.52	5905.84	14672.69	20578.53	5914.68	14673.07	20587.75	5923.52	14673.45	20596.97
7.05	2527.30	8066.40	10593.70	2533.22	8067.51	10600.73	2541.17	8068.78	10609.95	2549.12	8070.06	10619.18
8.95	577.719	3308.30	3886.02	582.05	3308.59	3890.63	590.70	3309.16	3899.85	599.35	3309.73	3909.07
11.38	423.95	1809.30	2233.25	428.33	1809.56	2237.89	437.09	1810.04	2247.11	445.82	1810.51	2256.33
12.84	395.58	1800.57	2196.15	399.79	1801.38	2201.17	408.22	1804.84	2213.06	416.65	1807.26	2223.91
13.63	386.86	1797.96	2184.82	391.19	1798.24	2189.43	399.85	1798.80	2198.65	408.51	1799.36	2207.87
15.70	770.92	4411.80	5182.72	775.21	4412.13	5187.33	783.78	4412.77	5196.56	792.35	4413.42	5205.78

TABLE VIII
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANOWHISKERS AND THIRTY ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =30)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}	E_{kin}	E_{pot}	E_{total}
5.92	277.22	34230.06	34507.29	281.87	34233.02	34514.89	291.18	34237.00	34528.18	300.48	34241.49	34541.96
6.63	277.22	19899.23	20176.45	281.87	19899.87	20181.75	291.18	19899.88	20191.05	300.48	19907.18	20207.66
7.05	277.22	10165.22	10442.44	281.87	10165.84	10447.71	291.18	10166.88	10458.05	300.48	10170.65	10471.13
8.95	277.22	3630.38	3907.60	281.87	3630.96	3912.84	291.18	3631.28	3922.46	300.48	3629.806	3930.28
11.38	277.22	1969.04	2246.26	281.87	1969.16	2251.03	291.18	1969.32	2260.49	300.48	1969.78	2270.26
12.84	277.22	1940.31	2217.53	281.87	1943.23	2225.10	291.18	1943.23	2234.41	300.48	1953.83	2254.31
13.63	277.22	1921.57	2198.79	281.87	1921.57	2203.45	291.18	1921.61	2212.79	300.48	1921.66	2222.14
15.70	277.22	4930.26	5207.48	281.87	4930.46	5212.33	291.18	4930.86	5222.04	300.48	4931.05	5231.53

TABLE IX
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANOWHISKERS AND FORTY ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =40)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
7.51	3945.45	12964.85	16910.29	3950.38	12965.26	16915.64	3961.43	12966.08	16927.51	3972.48	12966.91	16939.39
9.56	877.34	3010.69	3888.03	882.68	3011.13	3893.81	893.57	3012.12	3905.69	904.47	3013.10	3917.57
10.84	607.97	2228.56	2836.54	613.42	2229.00	2842.41	624.37	2229.93	2854.29	635.318	2230.85	2866.17
11.95	751.51	2879.45	3630.95	757.03	2879.86	3636.89	757.03	2879.86	3636.89	768.09	2880.68	3648.77
12.91	1043.06	3631.63	4674.69	1048.67	3631.96	4680.62	1059.89	3632.61	4692.50	1071.11	3633.27	4704.38
14.00	1424.59	5440.42	6865.02	1430.17	5440.78	6870.96	1441.33	5441.50	6882.84	1452.49	5442.22	6894.71
15.01	1619.26	6941.72	8560.98	1624.65	6942.27	8566.92	1635.41	6943.39	8578.80	1646.18	6944. 50	8590.68
16.46	1857.19	8130.09	9987.29	1862.93	8130.44	9993.37	1874.34	8130.90	10005.24	1882.58	8131.44	10010.02

TABLE X
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANOWHISKERS AND FORTY ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =40)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
7.51	357.07	16453.10	16810.17	363.06	16455.59	16818.65	375.04	16458.91	16833.95	387.02	16461.13	16848.16
9.56	357.07	3535.46	3892.53	363.06	3535.87	3898.93	375.04	3536.27	3911.32	387.02	3536.65	3923.67
10.84	357.07	2494.07	2851.14	363.06	2494.54	2857.60	375.04	2494.32	2869.36	387.02	2492.69	2879.71
11.95	357.07	3282.62	3639.69	363.06	3282.73	3645.79	375.04	3282.91	3657.96	387.02	3283.69	3670.71
12.91	357.07	4326.12	4683.18	363.06	4326.61	4689.67	375.04	4327.28	4702.32	387.02	4327.57	4714.59
14.00	357.07	6503.49	6860.56	363.06	6503.48	6866.54	375.04	6506.15	6881.19	387.02	6507.07	6894.10
15.01	357.07	8210.48	8567.54	363.06	8217.80	8580.86	375.04	8218.61	8593.65	387.02	8220.86	8607.89
16.46	357.07	9645.50	10002.57	363.06	9646.86	10009.91	375.04	9649.67	10024.71	387.02	9652.92	10032.95

TABLE XI
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY LANGEVIN DYNAMIC SIMULATION FOR SnO_2 NANOWHISKERS AND FIFTY ETHANOL MOLECULES

Langevin Dynamic (N. C_2H_5OH molecular =50)												
)istance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
6.31	11626.27	27714.50	39340.77	11632.91	27715.25	39348.17	11646.13	27716.63	39362.76	11659.36	27718.00	39377.36
9.76	15044.78	22380.49	37425.27	15051.69	22380.88	37432.57	15065.52	22381.64	37447.16	15079.33	22382.42	37461.75
10.22	15007.18	20758.14	35765.32	15013.95	20758.67	35772.61	15027.49	20759.72	35787.21	15041.02	20760.78	35801.80
11.42	1362.77	5838.11	7200.88	1369.74	5838.42	7208.16	1383.67	5839.05	7222.73	1397.60	5839.69	7237.29
13.57	2606.07	10739.32	13345.38	2613.19	10739.49	13352.68	2627.42	10739.85	13367.27	2641.65	10740.26	13381.91
14.95	3250.99	13816.66	17067.65	3258.01	13816.93	17074.94	3272.05	13817.48	17089.53	3286.09	13818.04	17104.13
16.52	3555.28	15705.05	19260.33	3561.95	15705.68	19267.63	3575.30	15706.92	19282.23	3588.66	15708.17	19296.82
17.47	4291.55	16562.65	20854.20	4298.78	16562.71	20861.49	4313.24	16562.85	20876.08	4327.68	16563.00	20890.67

TABLE XII
THE TOTAL ENERGY, POTENTIAL ENERGY AND KINETIC ENERGY (KCAL/MOL) CALCULATED IN DIFFERENT DISTANCES AND TEMPERATURES BY MONT CARLO SIMULATION FOR SnO_2 NANOWHISKERS AND FIFTY ETHANOL MOLECULES

Mont Carlo (N. C_2H_5OH molecular =50)												
Distance A^0	**298K**			**303K**			**313K**			**323K**		
	E_{kin}	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**	**E_{kin}**	**E_{pot}**	**E_{total}**
6.31	438.71	38910.60	39349.31	446.07	38911.56	39357.63	460.79	38912.73	39373.52	475.52	38913.74	39389.26
9.76	438.71	34798.21	35236.93	446.07	34800.76	35246.84	460.79	34803.72	35264.52	475.52	34900.20	35375.71
10.22	438.71	33463.73	33902.44	446.07	33452.33	33898.40	460.79	33419.87	33880.66	475.52	33390.68	33866.19
11.42	437.71	6756.56	7194.37	446.07	6756.91	7202.07	460.79	6759.04	7218.89	475.52	6761.44	7235.98
13.57	438.71	12911.22	13349.93	446.07	12911.80	13357.87	460.79	12914.48	13375.28	475.52	12919.10	13394.61
14.95	438.71	16621.19	17059.90	446.07	16622.07	17068.14	460.79	16624.08	17084.87	475.52	16626.61	17102.13
16.52	438.71	18833.22	19271.93	446.07	18844.89	19290.96	460.79	18849.98	19310.77	475.52	18851.61	19327.12
17.47	438.71	20367.98	20806.69	446.07	20369.63	20815.70	460.79	20371.96	20832.75	475.52	20586.88	21062.39

A. Discussion

The total energy, potential energy and kinetic energy calculated for interaction SnO_2 nanowhiskers and different number of ethanol molecules in different distance and temperatures. The calculations are shown in Tables I-X that with addition number of ethanol molecules and temperature of ethanol increased the energies. Fig. 4 are show the total energy decreased with addition distance mean of ethanol molecules related to SnO_2 nanowhiskers in initial so it increased with more addition distance mean of ethanol molecules. This decrease and increase the total energy with difficult mean of distances is more regular than with increase number of ethanol molecules.

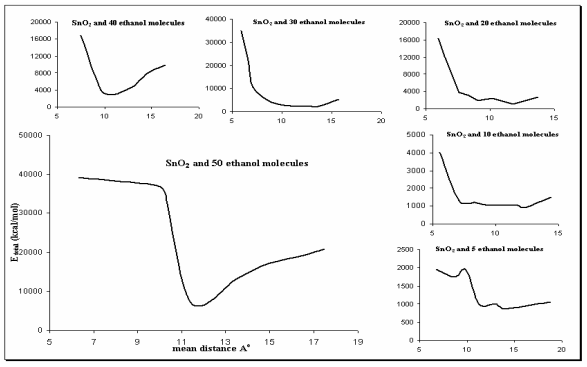

Fig. 4 The total energy (kcal/mol) calculated for interaction SnO_2 and ethanol molecules in different mean distance (A^o) at 298K by Langevin Dynamin simulation

The energies calculated by Langevin Dynamic and Mont Carlo simulation that was shown in Tables I-X. The trajectories obtained applying this algorithm agrees with those obtained by Langevin dynamic simulations. The efficiency of a Monte Carlo-based search engine depends on the interplay of the energy update protocol and the type of conformational movements used to modify a given conformation.

The total energy and potential energy are approximating same in both methods with addition distance mean. Therefore kinetic energy is changed with addition distance for method of Langevin Dynamic but it is same for Mont Carlo simulation.

B. Conclusion

The total energy depends linearly on the temperature, that it increase with addition temperature so this interaction is endothermic.

The total energy with two methods was decreased in initial so it was increased with addition distance mean that have indicated interaction between SnO_2 nanowhiskers and different number of ethanol molecules so it increased with addition number of ethanol molecules.

The diffusion behavior can be clearly distinguished as either normal-mode or single file mode in time scales of about 1000 ps. It is possible to show that setting a threshold of 1° on the movement of the dihedrals of the them backbone in a single Monte Carlo step, the mean quantities associated with the off-equilibrium dynamics are well reproduced, while the good description of higher moments requires smaller moves.

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