



Thermodynamic Properties of N₂ and O₂ (Molecular Dynamics Simulation)

M. A. B. A. ^{a,*}, M. Q. ^b, L. A. D. S. ^d, M. y. M. a. -R. c. a. d. ^b

^a Universidade Federal do Rio de Janeiro, ^b Universidade Federal do Rio de Janeiro, ^c Universidade Federal do Rio de Janeiro, ^d Universidade Federal do Rio de Janeiro

Received: 10/01/2024
Accepted: 15/01/2024
Published: 20/01/2024
Keywords: Molecular Dynamics, Thermodynamic Properties, N₂, O₂, Simulation

1. Introduction

Hybrid simulation methods combining molecular dynamics (MD) and Monte Carlo (MC) techniques have been widely used to study the thermodynamic properties of complex systems. In this work, we investigate the thermodynamic properties of N₂ and O₂ molecules using a hybrid MD/MC approach. The simulation results are compared with experimental data and theoretical predictions. The study is organized as follows: Section 1 presents the introduction, Section 2 describes the simulation methodology, Section 3 shows the results and discussion, and Section 4 concludes the work.

S... b e d c ... d a ... y b d s a ... d c e
a b ... e a y d ... c M a a d (A ...) a d
e a ... -d ... c ... a d e c e (R y ... a., 1994). C a e e
c d ... e y b d s a ... b ... M a a d e a d M ... ca
D c e (A. ...) a a ca e d ... e c e b
d c a d c ... e c f i c (A O U, 1983). T H a a a D c (A. ...)
e c ... y c a e f i d a e E d a ... d by I U C N R d L e (B d L
I ... a ... a., 2017) a y d ... c e e b d ... d c d
M a a d e A ... ca B a c D c (A. ...) b e a b
a y d c d d ... y b d s a ... M a a d e (K b y ... a.,
2004). I N Z a a d a d L d H ... I s a d, y b d s a ...
a G y D c (A. ...) M a a d e a e a y d c d
... a ... e ... G y D c e (W ... a ... s, 2017)
... e c e e ... b ... t c a ... c ... (T a c y ... a.,
2008; G a y ... a., 2015). I N Z a a d, M a a d ... y e
a e d c ... a e ... b ... d c e ... y b d ... y ... c a e e
(G ... e ... , 1985). C ... y, ... d M a a d e a d M a a d G y D c
y b d e a ... e c ... a d d e a d e c e s, a ... -
a ... y 500,000 d d a e b ... d a c y a (M c D ... a ... a d
A ... d e ... , 2017). T ... s ... t ... a ... s c e e
a d c d c ... f i ... d ... e ... b ... a c a b c a e ... d f f i c ... y
d e ... e b ... -M a a d, y b d e a d ... -G y D c e
(M ... t ... , 2008; W ... a ... s, 2017). T ... y b d s a ... M a a d a d G y
D c e ... t ... a ... d d a ... y ... a a e ... e c ...
... c ... a c a d a y a ... e ... t ... d ... a e ... t a ... y ... e
... t ... c a e e ... e e a d / ... y ... c ... -
c ... e ... t ... a ... s H ... , b ... e ... e c e ... a ... d c e
... d ... a ... a ... ca (J ... e ... a., 1999), ... t ... a ... e d e
... a ... a d f f e ... (K a , 1970), ... , a ... e e ... t c
... b ... c d ... b ... a ... y f f e ... a e a ... e
... c ... d a ... DNA (... DNA). T ... , ... y ... e ... a
a ... N Z a a d ... t a ... G y a d M a a d D c e a

the area of the fly (O'Connell, 1977; Yeh-Tsai, 2006). Nucleic acid extraction and PCR amplification of the DNA were performed as described in A. ... (Tab. 2)

d c a a y a a + y a s 0.4% CO1 a d 3.1%
+ c +).

עד עכשיו דא פארען ער דארט אדער א
-c d ע פארען 2-

García, A.A., Saares, B.J., Gaillard, T.D., 2014. A review of the (Palaearctic) *A. caudata* complex (Diptera: Cecidomyiidae) in North America. *Ann. Entomol. Soc. Am.* 107, 598–608.

Gay, P.-J., Winters, M., Riebel, R.W., 2015. Life history and biology of the *A. caudata* complex (Diptera: Cecidomyiidae) in North America. *J. Econ. Entomol.* 48, 103–109.

Hart, M.S., Suda, P.D., Vahana, F.X., Sadtler, T.A., Danks, J.W., Nadler, S.A., 1994. Description of a new species of *A. caudata* complex (Diptera: Cecidomyiidae) from South America. *Ann. Entomol. Soc. Am.* 87, 1087–1090.

Hart, B.D., Riebel, H.A., O'Byrne, D.J., 2000. The *A. caudata* complex (Diptera: Cecidomyiidae) in North America. *J. Econ. Entomol.* 33, 78–79.