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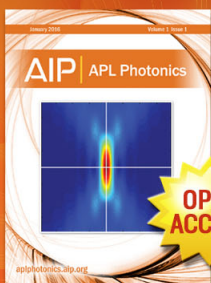
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## Head-disk interface design in magnetic data storage

Sesha Hari Vemuri,<sup>1</sup> Pil Seung Chung,<sup>1</sup> Robert L. Smith,<sup>1</sup> Nae-Eung Lee,<sup>2</sup> Lorenz T. Biegler,<sup>1,2</sup> and Myung S. Jhon<sup>1,2,a)</sup>

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Superior electrical conductivity and thermo-mechanical response of graphene can significantly improve areal density in magnetic data storage. The current head media spacing in hard disk drives (HDD) is 7.2 nm, and replacing conventional carbon overcoat (COC) with graphene will drastically reduce head media spacing, increasing areal density to eight times its present value. A paradigm shift in HDD systems can also be achieved via selection of a combination of new lubricants and unconventional architecture of COC systems. Here, we evaluate the feasibility of graphene overcoat (GOC), by understanding GOC-lubricant interactions. We further introduce new alternative head-disk interface (HDI) designs consisting of buffer/lubricant layers (i.e., graphene/carbon nanotube (CNT) or fullerene/perfluoropolyether (PFPE)). These hybrids could further enhance tribological performance including the reduction of wear and friction while drastically increasing areal density of data storage devices. Our study here will lead to vigorous investigation of HDI in magnetic data storage, including heat-assisted magnetic recording (HAMR), with tuned atomistic design criteria. © 2012 American Institute of Physics. [doi:10.1063/1.3679464]

### INTRODUCTION

Hard disk drives (HDDs) have been the dominant devices for data storage in recent history. In order to bring a paradigm shift in HDD systems, our focus is now geared toward the head media spacing (HMS), specifically the carbon overcoat (COC). Many studies have been performed on lubricant materials, which are primarily perfluoropolyether (PFPE) oligomers, to analyze the surface coverage and self-healing properties.<sup>1</sup> However, a thorough understanding of the molecular structures of these lubricants from an intermolecular perspective simultaneously with study of the COC is necessary to construct accurate multi-scale models. Thus, there is a need for atomistic models to reveal the interaction behavior of each PFPE molecule with COC.

The properties of graphene,<sup>2–4</sup> including superior electrical conductivity and excellent thermo-mechanical response, will revolutionize many nano devices and potentially improve areal density in HDDs, as shown in this paper. Current head media spacing is approximately 7.2 nm to achieve 1 Tb/in<sup>2</sup> (Fig. 1(a)), and using a graphene overcoat (GOC) will drastically reduce HMS (Fig. 1(b)),<sup>5</sup> increasing areal density by as much as eight times its current value based on milestones achieved so far.<sup>6</sup> This is a significant improvement in HDD simply by reducing COC thickness alone. Thus, it is of extreme importance to understand GOC-PFPE interactions at the most fundamental level.

We specifically perform *ab initio* simulations of the interaction between functional PFPE oligomers and GOC from a qualitative viewpoint. The role of the COC is brought to light

by performing a feasibility study on graphene without changing the chemical structures of the lubricants. The methodology proposed here can be used as a foundation for higher level descriptions in a multi-scale scenario, including bead spring models,<sup>7–9</sup> where clusters of atoms are represented by single lower resolution sites in molecular dynamics simulations. Here, we focus on the establishment of the foundations for coarse-graining of the lubricant models so that mesoscale phenomena can be observed via molecular dynamics methods. Further, we introduce the concept of solid state buffer layers to reinforce the GOC layer.

### THEORETICAL METHODS

In our model, three examples of PFPEs are analyzed: Zdol, Ztetraol, and Demnum di-propyl amine (DDPA), the chemical structures of which are given in Fig. 1(c). The atomistic modeling of PFPEs with extensive *ab initio* computations presents a significant challenge. As a consequence, we have idealized PFPE chemical structure by truncating the entire molecule to a structure containing the functional group, which is expected to primarily contribute to the interaction with other endgroups and the GOC. The DDPA is modeled by focusing on the propyl groups and nitrogen atom, resulting in a simple yet realistic calculation of interaction energies of DDPA with graphene. The interaction energies of each individual GOC-PFPE dimer in the above mentioned test cases are examined.

Calculations have been performed in Q-Chem 3.2 (Ref. 10) at the Hartree-Fock level of theory with the Dunning correlation consistent polarizable valence double zeta (cc-pVDZ) basis set. The uncorrected interaction energy

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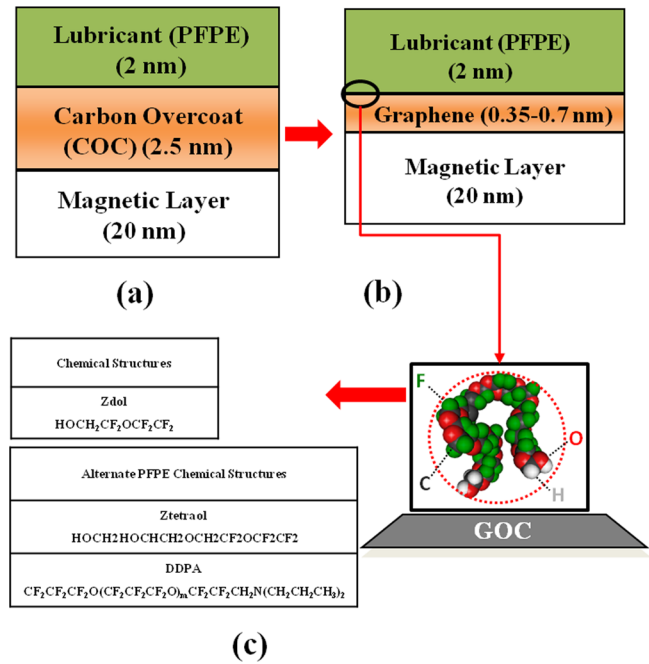


FIG. 1. (Color online) (a) Existing specs of media interface, (b) specs with graphene overcoat, and (c) an atomistic view of PFPE-GOC.

TABLE 1. The uncorrected and counterpoise corrected interaction energies for lubricant-GOC clusters for single layer [denoted as (s)] and double layer [denoted as (d)] graphene

PFPE	$E_{\text{int}}^{\text{CP}} \text{ (s)}$ (kcal/mol)	$E_{\text{int}}^{\text{CP}} \text{ (d)}$ (kcal/mol)
Zdol	−1.85	−2.43
Ztetraol	−1.46	−5.98
DDPA	−0.405	−3.91

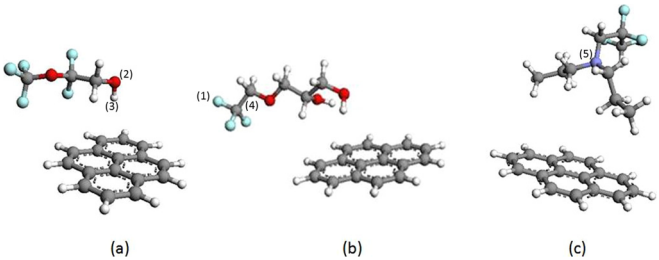


FIG. 2. (Color online) (a) Zdol-graphene equilibrium geometry, (b) Ztetraol-graphene equilibrium geometry, and (c) DDPA-graphene equilibrium geometry. Red: oxygen, violet: nitrogen, blue: fluorine, gray: carbon, and white: hydrogen.

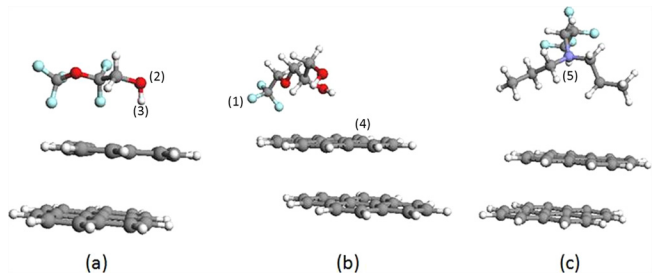


FIG. 3. (Color online) Two layer graphene with (a) Zdol, (b) Ztetraol, and (c) DDPA. Red: oxygen, violet: nitrogen, blue: fluorine, gray: carbon, and white: hydrogen.

represented by the potential energy of the configuration is calculated as:

$$U_{\text{int}} = U_{(\text{A-B})} - U_{\text{A}} - U_{\text{B}}, \quad (1)$$

where  $U_{(\text{A-B})}$  is the energy of the dimer and  $U_{\text{A}}$  and  $U_{\text{B}}$  are the energies of isolated monomers A and B, respectively.

The finite basis sets used in the calculations cause each monomer to share basis functions with other monomers in the dimer calculation, which is known as basis set superposition error (BSSE). As a consequence, the interaction energy is overestimated by Eq. (1). Thus, to reduce the BSSE associated with our computational techniques, a counterpoise correction (CP) is used for Eq. (1):

$$U_{\text{int}}^{\text{CP}} = U_{\text{int}} + \text{BSSE} \\ \text{BSSE} = U_{(\text{A-0})} - U_{(\text{A-X})} + U_{(\text{B-0})} - U_{(\text{B-X})} \quad (2)$$

where  $U_{(\text{A-0})}$  is the energy of monomer A at the dimer geometry and  $U_{(\text{A-X})}$  is the energy of monomer A at the dimer geometry with the added basis functions of monomer B, with an analogous treatment for monomer B.

The above procedure was adopted for the GOC-PFPE interaction simulations, where graphene was modeled as a single nanoflake with edges passivated with hydrogen to stabilize dangling bonds. As a result of the limitations of our computational method, we use a clustered lubricant-graphene calculation, therefore, our model graphene includes edges which, preserves the  $\text{sp}^2$  hybridization of the carbon atoms. A similar study demonstrated that when comparing adsorption on graphene with and without periodic boundary conditions, there is no qualitative change in the adsorption behavior.<sup>11</sup>

## RESULTS AND DISCUSSION

Table I shows the interaction energies of PFPE-GOC dimers, where a negative value denotes attraction, and a positive value denotes repulsion. Figure 2 illustrates the relaxed structures of Zdol, Ztetraol, and DDPA with GOC. The frequency analyses of all dimer complexes produced no imaginary frequencies, ensuring a minimum on the potential energy surface, rather than a transition state or saddle point. For the hydroxylated endgroups, the closest intermolecular bond with a graphene carbon is formed with the OH group hydrogens. For Zdol, this bond length is 2.79 Å, and the bond length between Ztetraol's secondary OH group and a graphene carbon is 2.92 Å. Conversely, the shortest intermolecular bond between a graphene carbon and DDPA's propyl group hydrogen is 3.58 Å. The shorter intermolecular bond lengths for the hydroxylated endgroups point toward stronger interactions with graphene when compared with DDPA. The interaction energy results in Table I indicate that all of the endgroups have stable interactions with the model graphene. However, DDPA's interaction energy with the GOC is still much lower compared to Zdol and Ztetraol, which is consistent with the intermolecular bond length results. These qualitative findings indicate that all of the lubricants may have the capability to adhere to a graphene surface, although a more

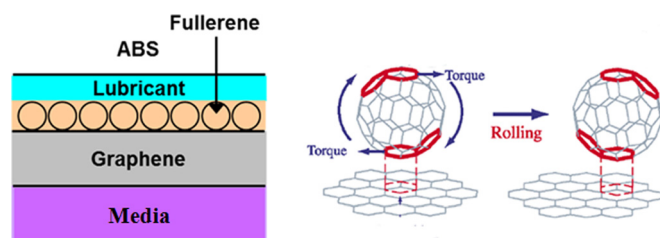


FIG. 4. (Color online) A schematic of the HDI with fullerene buffer layer between the PFPE lubricant and graphene. The motion of the fullerene on graphene can provide additional lubrication.

weak adhesion is observed for DDPA, making it a less suitable candidate for the lubrication of GOC, while Zdol could be the most preferred candidate.

In order to further protect the storage media, an additional layer of graphene may be necessary to provide practical protection. To evaluate the effect of having a two-layer graphene surface on lubricant adhesion, an additional layer was added to the lubricant-GOC dimers in Fig. 3. The additional layer was added at the experimental graphene-layer separation of 3.35 Å, and the interaction energy of the lubricant at this geometry (shown in Fig. 3) was calculated. Table I shows the lubricant adhesion improves with the introduction of the second layer, particularly for the Ztetraol and DDPA forms. Ztetraol adhesion improves by a factor of 3, while we observe a factor of 5 improvement in DDPA's interaction with the GOC. Thus, in addition to the extra protection to the magnetic media offered by an additional layer of graphene, our calculations indicate more desirable lubricant adhesion can be achieved as well.

In addition to the lubricant surface adhesion, the lubricant self-healing property is an additional design criterion that must be considered. In order to find the most suitable candidate, the introduction of systematic nanoblending of PFPE may be necessary to find the optimal PFPE composition. Further, large size graphene sheet interaction with PFPEs along with significant defects including grain boundaries is currently being investigated. We are in the process of evaluating three-body interactions between PFPE dimers and larger graphene nanostructures to make a linkage with molecular/meso scale models. At the molecular/meso scale, coarse-graining procedures will be used, taking input from our atomistic simulation.

When considering graphene as a COC replacement, its atomically thin structure is an advantage for areal recording density, but the thin structure may need additional reinforcement to adequately protect the media layer. As shown in Fig. 4, one might examine the concept of a solid state buffer layer to cover the graphene surface. Candidates for the buffer material include various fullerenes (e.g., carbon nanotubes,

C<sub>60</sub>) because the friction with graphene would be small and the overall thickness would still be an improvement over current carbon overcoats.<sup>12</sup> In the event of an applied torque during slider contact, additional lubrication could be offered by the solid buffer. We are currently investigating the interaction between PFPE lubricant and fullerene structures to evaluate the feasibility of a PFPE-buffer-graphene hybrid system with various combinatorial configurations.

## CONCLUSIONS

We calculated interaction energy with *ab initio* methods for model PFPE-GOC dimers. By our atomistic scale investigation, we have demonstrated a qualitative trend in endgroup structure influence on adsorption on graphene. Our feasibility study indicates graphene could replace existing COC when using conventional lubricants like Zdol and Ztetraol due to significant adhesive properties, and they may be superior to new lubricant materials like DDPA. However, Ztetraol and DDPA exhibit much stronger adhesion with the addition of a second layer. We further introduced the concept of a solid state buffer layer between PFPE and graphene to add extra lubrication and protection of the GOC. Our study will eventually lead to investigation on the PFPE-PFPE and PFPE-COC interactions that can be tuned to develop atomistic design criteria in lubricant technology.

## ACKNOWLEDGMENTS

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- <sup>1</sup>P. S. Chung and M. S. Jhon, *IEEE Trans. Magn.* **46**, 2405 (2010).
- <sup>2</sup>K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, *Science* **306**, 666 (2004).
- <sup>3</sup>D. W. Boukhvalov and M. I. Katsnelson, *J. Phys.: Condens. Matter* **21**, 344205 (2009).
- <sup>4</sup>V. Barone, O. Hod, and G. E. Scuseria, *Nano Lett.* **6**(12), 2748 (2006).
- <sup>5</sup>B. A. Gurney, E. Marinero, and S. Pisana, U.S. patent application # US2011/0151278A1 (2011).
- <sup>6</sup>B. Marchon and T. Olson, *IEEE Trans. Magn.* **45**, 3608 (2009).
- <sup>7</sup>P. S. Chung, H. Park, and M. S. Jhon, *IEEE Trans. Magn.* **45**, 3644 (2009).
- <sup>8</sup>H. J. Choi, Q. Guo, P. S. Chung, and M. S. Jhon, *IEEE Trans. Magn.* **43**, 903 (2007).
- <sup>9</sup>R. Smith, P. S. Chung, J. A. Steckel, L. T. Biegler, and M. S. Jhon, *J. Appl. Phys.* **109**, 07B728 (2011).
- <sup>10</sup>C. A. Kong, A. I. White, C. D. Krylov, R. D. Sherrill, T. R. Adamson, M. S. Furlani, A. M. Lee, S. R. Lee, T. R. Gwaltney, C. O. Adams, A. T. Chsenfeld, B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople, *J. Comput. Chem.* **21**, 1532 (2000).
- <sup>11</sup>C. Thierfelder, M. Witte, S. Blankenburg, E. Rauls, and W. G. Schmidt, *Surf. Sci.* **605**, 746 (2011).
- <sup>12</sup>K. Minura, S. Kamiya, and N. Sasaki, *Phys. Rev. Lett.* **90**, 055509 (2003).