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Adaptive Infrastructure under Climate Change

Properties of Polymer Modified Asphalt by Polyphosphoric Acid at High-temperatures

Yujie Tang, Chang 'an University, yujietang2022@chd.edu.cn
Zhen Fu, Chang 'an University, zhenfu@chd.edu.cn
Feng Ma, Chang 'an University, mafeng@chd.edu.cn

Introduction

Background:

Polymer (SBR in this study) modified asphalt could greatly improve performance of pavement and prolong its service life. Unfortunately, terrible stability and compatibility of SBR modified asphalt limited further large-scale application, especially in inferiority of high-temperature performance. As a low-cost chemical modifier, PPA could make up disadvantages of SBR modified asphalt due to it's excellent enhancement effects.

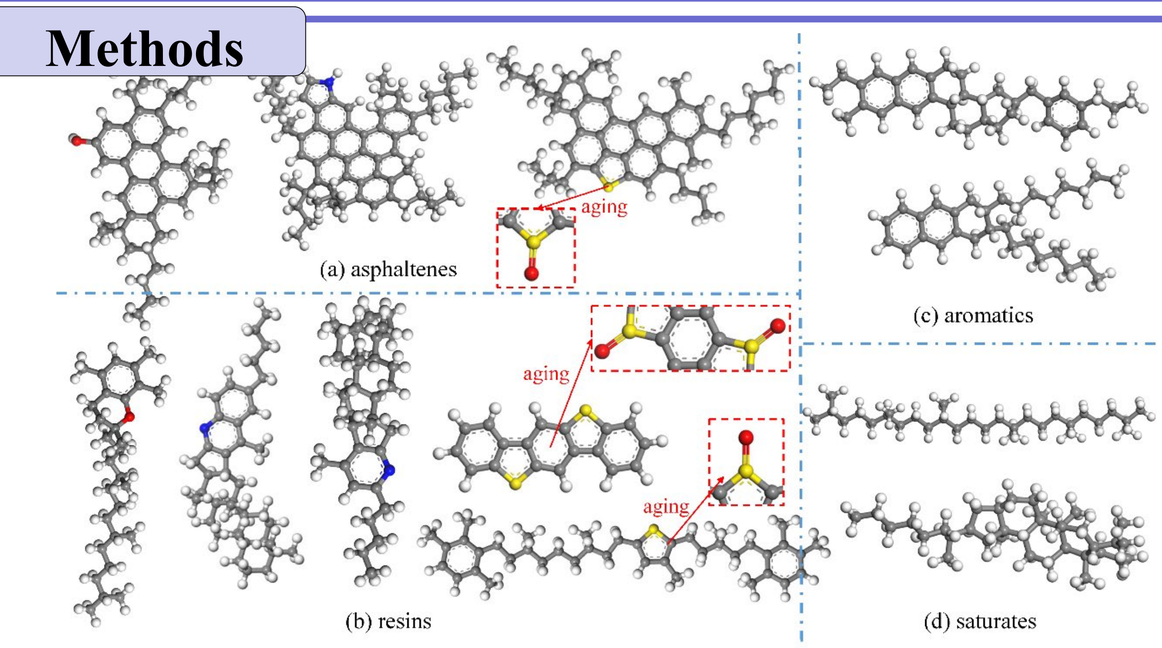
Research gap:

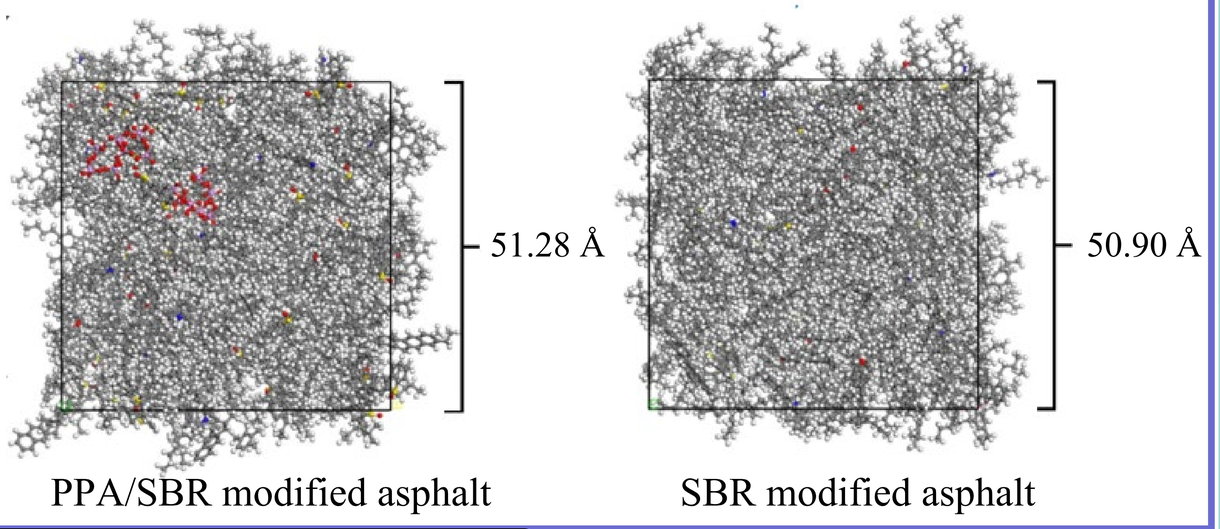
The majority of studies focused on test performance characterization but ignored theory explanation. The main breakthrough lies in modification and absorption mechanism of PPA in SBR modified asphalt.

Research aim:

This study investigated the molecular dynamics properties and modification mechanism of polyphosphoric acid (PPA) and styrene-butadiene rubber (SBR) composite modified asphalt binder by molecular dynamics simulation.

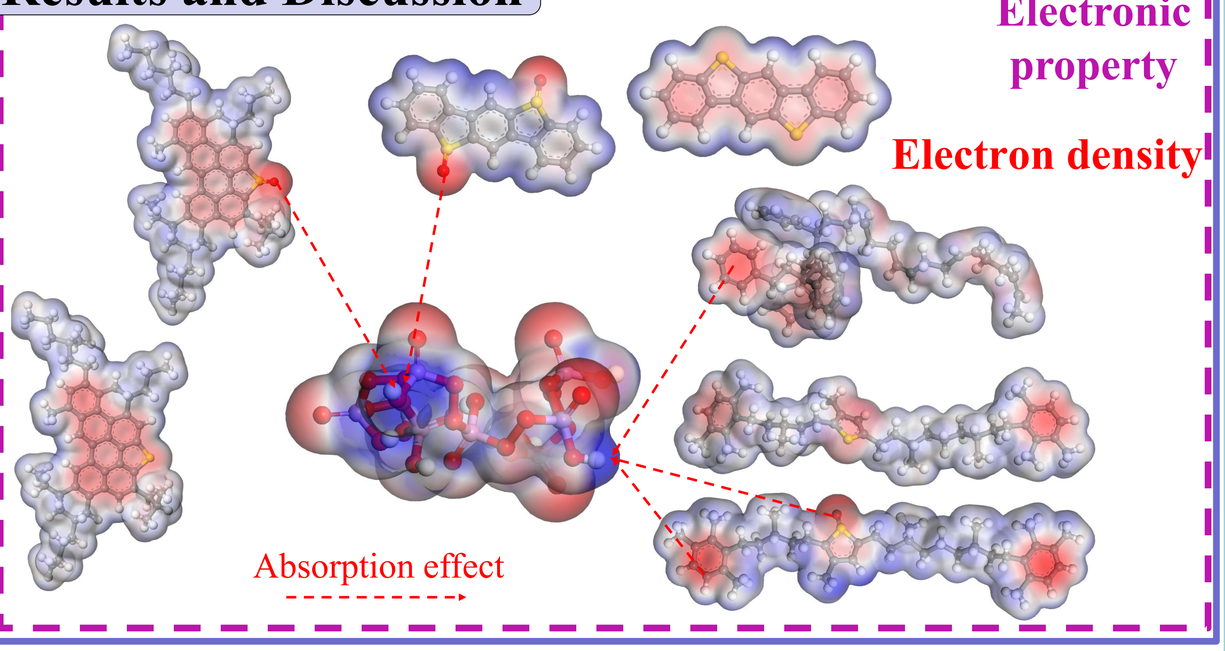
Methods



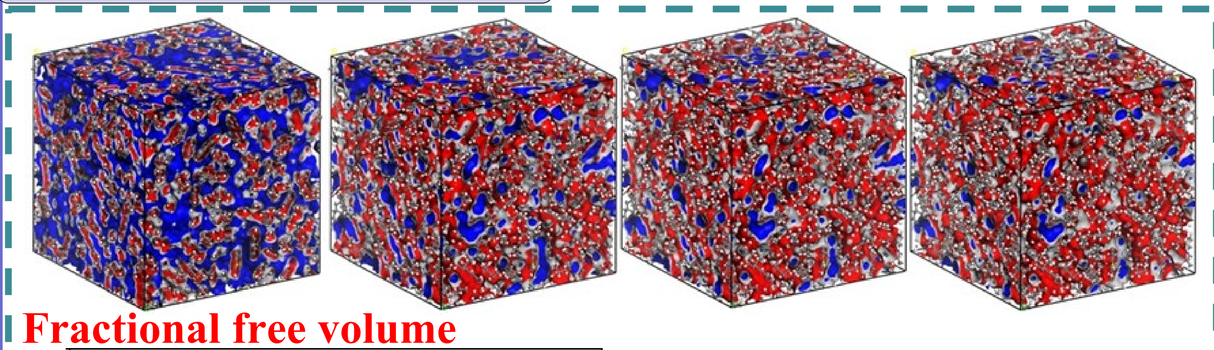


PPA/SBR modified asphalt SBR modified asphalt

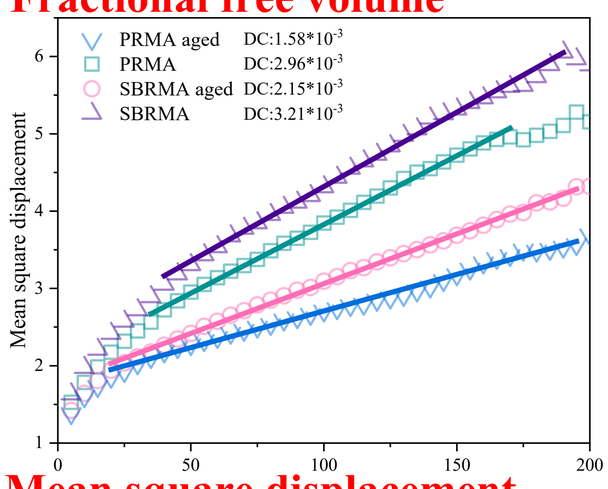
Results and Discussion



Results and Discussion



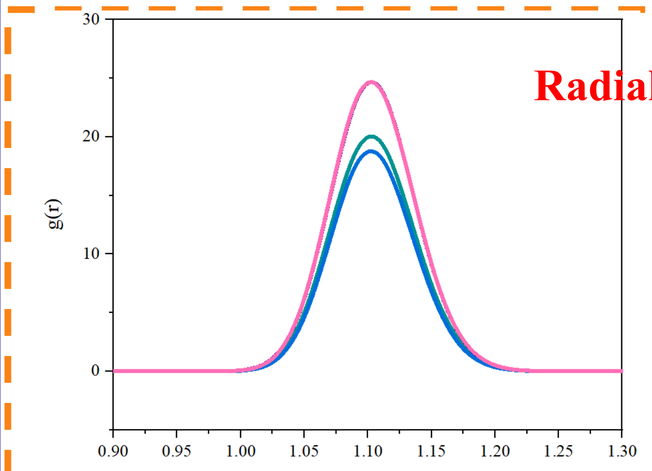
Fractional free volume

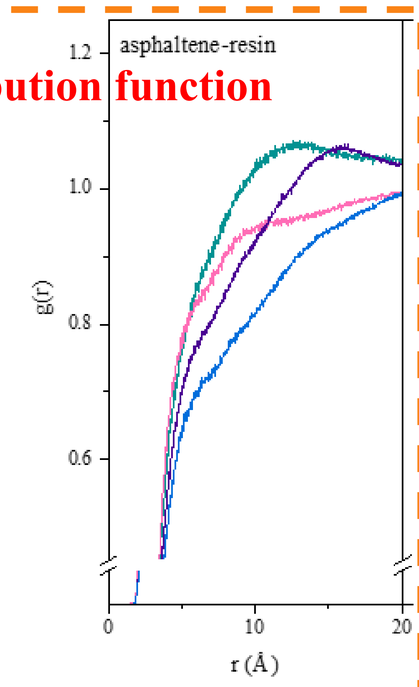


PPA ↑ Aging ↑
Free volume ↓
Mobility of molecules ↓
Diffusion ↓

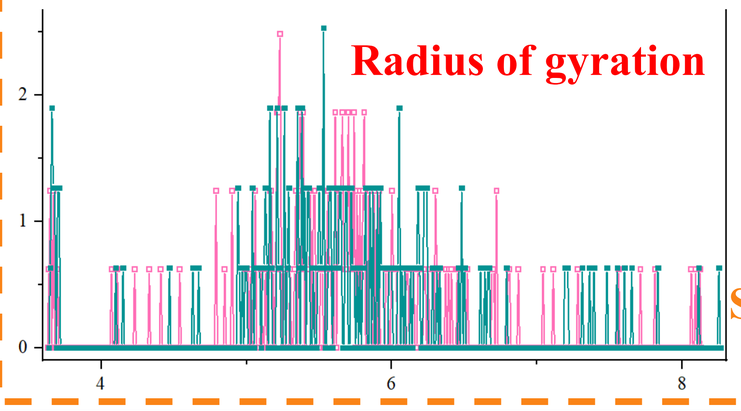
Mean square displacement — **Diffusion and mobility**

Radial distribution function





Radius of gyration



Stability and orderliness of molecular structure

Conclusion

Based on molecular dynamics simulation, the FFV and MSD of modified asphalt system showed that diffusion and mobility capability of asphalt binder weakened after aging or adding PPA. This meant PRMA or aged binder was difficult to deform because PPA could absorb asphalt molecules and the size and weight of PPA and aged asphalt molecules were larger than unaged asphalt molecules. The RDF and Rg revealed PPA and aged asphalt molecules had more stable and order molecular structures. The interaction between P=O/P-OH and S=O/aromatic rings made a better stability and orderliness of asphalt molecular structure. These results explained why PPA could enhance rutting resistance and stability at high temperatures at molecular-level view.

Acknowledgment

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