Improved dielectric properties and grain boundary effect of phenanthrene under high pressure

Xiaofeng Wang 1, Qinglin Wang 1\*, Tianru Qin 2, Guozhao Zhang1\*, Haiwa Zhang1, Dandan Sang1, Cong Wang3, Jianfu Li4, Xiaoli Wang4\*, Cailong Liu1

1Shandong Key Laboratory of Optical Communication Science and Technology, School of Physics Science and Information Technology, Liaocheng University, Liaocheng 252059, China

2Heilongjiang Province Key Laboratory of Superhard Materials, Department of Physics, Mudanjiang Normal University, Mudanjiang 157012, China

3College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing 100029, China

4School of Opto-electronic Information Science and Technology, Yantai University, Yantai 264005, China

**\* Correspondence:**Qinglin Wang, Guozhao Zhang, Xiaoli Wang
wangqinglin@lcu.edu.cn, Z2012GZ@163.com, and xlwang@ytu.edu.cn



**Fig. S1** Raman modes of *L*1 and *L*2 as a function of pressure. The solid lines are the linear fit to the data.



**Fig. S2** High pressure Raman spectra of phenanthrene and pressure dependence of the Raman shift in region of 2800-3250 cm-1. Dashed vertical lines represent phase boundaries, and phases are assigned with Roman numbers. (*ν*29, *ν*30) and (*ν*27, *ν*28, *ν*31) correspond to the symmetric and asymmetric stretching vibrations of the C-H bond, respectively.

**Table S1** The pressure dependence of intramolecular and intermolecular bond distances.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Phase | Intramolecular | d*L*Intra/d*P* (Å/GPa) | Intermolecular | d*L*Inter/d*P* (Å/GPa) |
| I | C24-C28 | -0.00087 | C18-H18 | -0.00042 |
| C26-C24 | -0.00150 |
| C16-C26 | -0.00150 |
| C18-C20 | -0.00062 | H18-H8 | -0.02800 |
| C28-C18 | -0.00049 |
| C16-C20 | -0.00100 |
| II | C46-C47 | -0.00160 | C44-C21 | -0.06100 |
| C47-C48 | -0.00210 |
| C45-C46 | -0.00160 | H32-H27 | -0.04100 |
| C44-C45 | -0.00160 |
| C48-C43 | -0.00130 | C44-H32 | -0.00087 |