

## Density-Functional Theory to Study of Polymeric Structures and Properties

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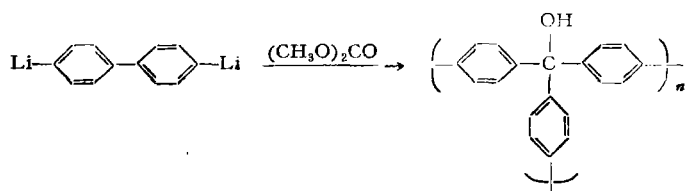
**Summary** With the progress of polymer science for much more theories the explanation of polymeric properties is sought out. This paper gives a introduction to density-functional theory which is pending further perfection but have many advantages, and has a review of applications of this theory to study of polymeric structures and properties. It is notice, however, that this subject has been just beginning. So many courses will be to study on.

**Key words** Density-Functional Theory, Polymer, Chemical Physics

### 超 交 联 树 脂

杜邦公司的Webster开始制作交联密度的聚合物时,原意是想做“有机沸石”,但实际上拿到的却是一种“白炭黑”,蓬松的粉末没有沸石的强度和耐高温性,但有非凡的表面积和化学活性使其别具用途。

例如Webster等人通过下列反应:



合成的聚合物,固体的碳-13核磁谱表明它具有完全的聚三芳基甲醇结构,一点儿甲氧甲酰基残余也没有。77°K时的氮吸附研究指出其比表面积是1167m<sup>2</sup>/g,孔容是0.79ml/g,孔径是2.8nm。由于它具有高度微孔,所以化学活性很高,比方说,用酸化的甲醇处理就生成甲醚,用氯化亚锡还原则给出聚三芳基甲烷,后者与三氟化硼-乙醚反应生成红色的聚三芳基碳鎓。虽然这种聚碳鎓在用碘化四丁基铵处理时释放出理论量80%的三碘化物来,但顺磁共振却没有测到自由基的讯号,可能是发生了偶合。这种聚三芳基甲烷也可以与丁基锂反应生成树脂状的聚负碳离子。

X-射线衍射研究表明它是无定形物质,在400℃的氮气中稳定。这种树脂能吸收其自身体积6倍的二氯甲烷而不湿,真可谓是“豪饮聚合物”。虽然交联密度这么高(每单体单元一个交联),但在溶剂润湿下仍能膨胀1倍,Webster对此的解释是交联微区之间形成了交联网。Webster还用类似反应合成了其它一些超交联的树脂,例如由碳酸二甲酯与三(4-锂苯基)胺反应得到的聚胺树脂,用乙酸处理时,会变成亮蓝色,令人想起诸如龙胆紫那样的三氨基三芳基甲烷类染料。

(郑 平 摘译自C&EN July 1, 1991, p.41~42)