Supporting Information

The molecular design of performance-enhanced intraocular lenses composite

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1. Clustering analysis

By performing a 500 *ns* MD simulations on the three IOLs model systems, the trajectory files contained 250000 frames. With the aid of clustering analysis, these frames were clustered into several groups. The structures in each group possessed the same structural characteristics as each other. The average-linkage algorithm[1] is used in the clustering analysis. In the process of clustering analysis, the structure represented by each frame represents its own cluster at the beginning of the analysis. Two clusters with close distances will be merged into the same cluster in the next iteration. During the iteration, if the required number of clusters *n* has been obtained (here *n* = 5), the calculations stops. The distance between cluster A and cluster B is defined as such: the average of all distances between a and b, where a (b) is a frame structure in cluster A (B). Through the clustering analysis, we can obtain a representative structure that represents each IOLs model, which will be used for subsequent IOLs model material performance simulating and testing.

2. Simulating the properties of the IOLs materials

Based on the IOLs models obtained through MD simulations and clustering analysis, the properties of the IOLs materials, such as the simulation of glass transition temperature (T_g), solvent accessible surface analysis and strain-stress analysis.

The glass transition temperature (T_g) refers to the temperature at which a polymer material changes from a glass state to a highly elastic state. The T_g is an inherent property of amorphous polymer materials. The glass transition temperature (T_g) can be investigated by MD simulations under NPT condition. By performing MD simulations

on IOLs model systems, the changes of the specific volume with temperature can be obtained. Thus, the value of T_g can be estimated from the slope of change.[2, 3] Here, the temperature ranges from 200 K to 400 K with an interval of 20 K were chosen. The well-equilibrated structures of three IOLs models obtained by MD simulations were used as the starting point for the T_g simulations. A time period of 50 ns simulation under NPT conditions was performed at each target temperature for the data collection.

In the fields of engineering and materials science, the stress-strain curve can be used to describe the relationship between the strain and the external force of a material under external compression (or tension). In a constant deformation rate experiment, there are usually five states of strain amplitude[4-6]:

1) linear stress growth in the low strain elastic regime;

2) when the strain exceeds a few percent, an "non-elastic" regime is entered, in which the stress increases more slowly than linearly;

3) the stress continues to increase, a local stress maximum at the so-called "yield peak", followed by a reduction in stress, a regime known as "strain softening";

4) a plastic flow regime characterized by a constant plateau stress;

5) finally, at large enough deformation the material either fails or the stress increases strongly due to chain deformation and "strain hardening".

For IOLs materials, the glistening is mostly caused by many "cavities" inside the material. In order to quantitatively characterize the internal "holes" of different IOLs materials, here we perform strain-stress analysis on these materials. It is not difficult to

understand that for a certain IOLs material, if there are many "cavities" inside, the structure will easily deform when external compression is applied to it. In comparison, if a certain IOLs material has fewer internal "cavities", its structure is less prone to deformation under the same external compression.

The stress-strain analysis for the IOLs models was conducted with the aid of the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[7]. In order to use the AMBER GAFF2 force field in LAMMPS, the InterMol software package[8] was employed for the format transfer from AMBER topology files to LAMMPS data files. The uniaxial compression simulation generated the stress-strain curves for IOLs models. By decreasing the z-direction dimension of the simulation box at a constant rate in the $N\sigma_x\sigma_y T$ ensemble, we can obtain the stress-strain curves. The deformation rate used in the simulation was $4.5 \times 10^{-3}\, ps^{-1}$.

3. Hydrogen bond analysis

Hydrogen bond analysis was performed on all the structures generated by MD simulations of all the IOLs models (Sensar AR40e, Acrysof SN60WF, enVista MX60 and Acrysof SN60WF-EG-DMA) in this study. In the present study, the following two criteria are employed to judge whether or not a hydrogen bond is formed between an acceptor heavy atom A, a donor hydrogen atom H and a donor heavy atom D. First, the distance between atom A and H is less than the distance cutoff 2.9 Å. Second, the A-H-D angle is greater than the angle cutoff $135.0°$. The hydrogen bonds between all the atoms inside the IOL models and the water

molecules inside IOL models were all monitored, the results of which are shown in Figure S3.
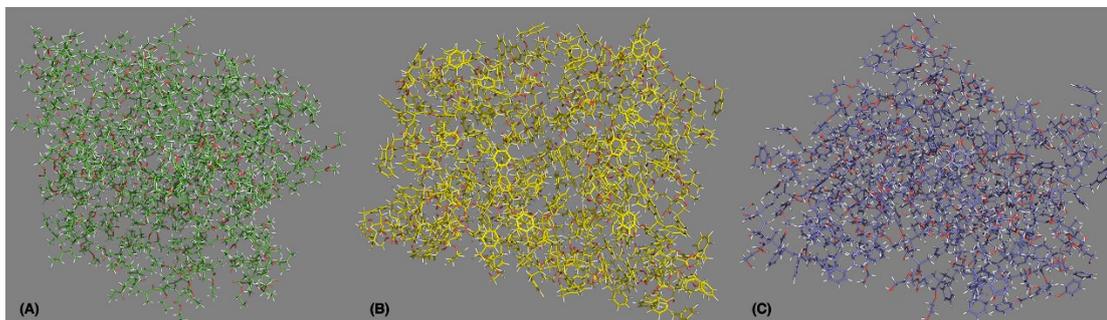
Figure S1. The model structures for (A) Sensar AR40e (carbon atoms in green), (B) AcrySof SN60WF (carbon atoms in yellow) and (C) enVista MX60 (carbon atoms in purple)
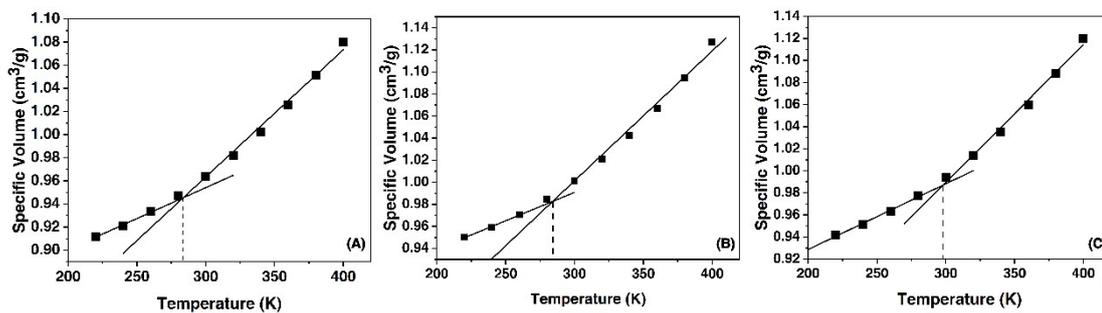
Figure S2. The dependence of the specific volume on temperature for (A) Sensar

AR40e, (B) AcrySof SN60WF and (C) enVista MX60. The cross of the two plots

corresponds to the glass transition temperature.
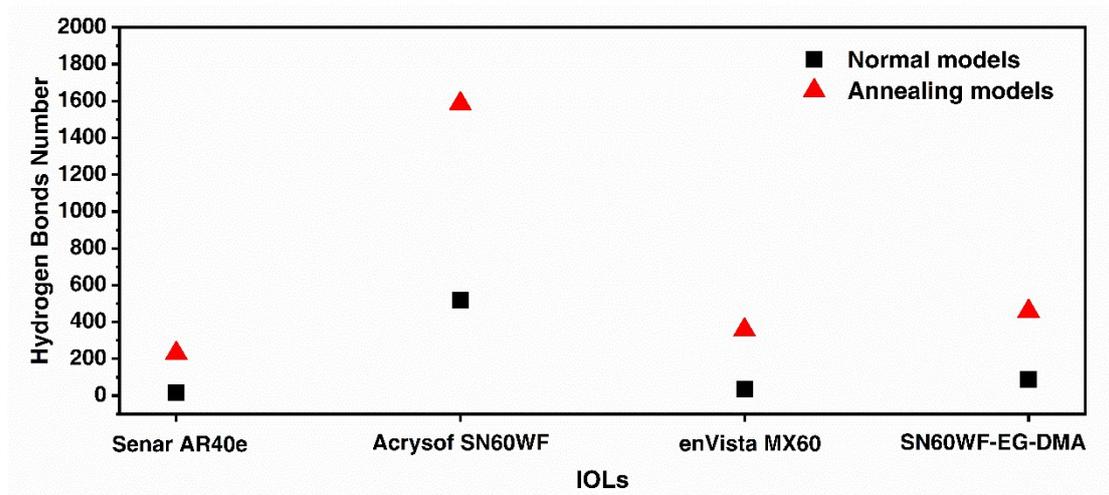
Figure S3. The number of hydrogen bonds formed inside the cavities of different IOLs for normal models (black dots) and annealing models (red dots).

Table S1. The simulated and the experimental glass transition temperature (T_g)

for the three IOLs in this study.

	Simulated T_g (K)	Experimental T_g (K)[9, 10]
Sensar AR40e	284	284 ~ 285.76
AcrySof SN60WF	285	287.15 ~ 288.65
enVista MX60	299	294.15

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