





**Fig. 3** UV spectra of **1** in water–ethanol mixtures (concentration of **1**: 10  $\mu\text{M}$ ). Inset: differential spectra of **1** ( $A$  and  $A_0$  being absorbance of **1** in mixture solvent and absolute ethanol, respectively).

The silole may exist mainly as a twisted conformer when it is molecularly dissolved in a good solvent. A twisted rotamer of **1**, whose energy was minimised by the MM2 method in a CS Chem3D Pro program, is given in Fig. 1. The phenyl peripheries linked to the silole core are obviously out of coplanarity. It has been proposed that coplanarisation of chromophores can be induced by aggregation.<sup>7</sup> When **1** aggregates, coplanarisation of its peripheries and core may be induced to a certain extent. It is well known that coplanar and twisted conformers have different resonance energy: when the rings are on the same plane, the degree of conjugation is at a maximum; when the rings rotate to 90° to one another, the conjugation drops to a minimum. The best-known example of this is biphenyl (**2**) and its non-coplanar 2,2'-dimethyl homologue (**3**), which exhibit quite different electronic properties (e.g.  $\epsilon_2/\epsilon_3 > 20$ ). The coplanarisation of **1** induced by the aggregation leads to a better conjugation between its peripheries and core, thus intensifying and red-shifting its absorption and emission bands. The silole molecules in the nanoaggregates cannot, however, assume a perfect coplanar conformation due to the involved steric crowdedness, and the phenyl rings may still rotate to some degree to cope with the steric repulsion. Such rotation will preclude co-facial alignment of the molecules and hinder excimer formation.<sup>7</sup> Aggregation quenching thus cannot operate in the luminescence process of **1**.

To further verify that aggregation quenching is not involved and to prove the usefulness of the novel luminescence property, we carried out a solid-state 'dilution' experiment and prepared a series of composite films of **1** and poly(methyl methacrylate) (PMMA). The compatibility of **1** and PMMA enabled us to cast thin films of optical quality from its chloroform solutions. The progressive red-shift of the PL spectrum with an increase in the content of **1** manifests the formation and population of the nanoaggregates in the solid 'solutions' (Fig. 4A). The linear increase of the luminance with the content of **1** testifies that the light emission is not quenched by aggregation. The composite film with 90% of **1** emitted a blue light of 492 nm with a high luminance of  $\sim 24000 \text{ cd m}^{-2}$ . We built an electroluminescence (EL) device of ITO/CuPc/TPD/**1**/Mg-Ag,<sup>†</sup> which emitted a blue light of 496 nm. When an  $\text{Alq}_3$ <sup>†</sup> layer was introduced, the device ITO/CuPc (20 nm)/TPD (50 nm)/**1** (50 nm)/ $\text{Alq}_3$  (10 nm)/LiF-Al showed a low turn-on voltage (3.4 V), high emission efficiencies ( $9234 \text{ cd m}^{-2}$ ,  $12.6 \text{ lm W}^{-1}$ , and  $12 \text{ cd A}^{-1}$ ) and external quantum yield (8%). When the thickness of the  $\text{Alq}_3$  layer was optimised (7 nm), the power efficiency was boosted to  $20 \text{ lm W}^{-1}$ . The silole is thus an excellent light-emitting material for the device application.



**Fig. 4** (A) PL spectra of **1**-PMMA composites (excited at 325 nm). (B) Luminance of the composite film vs. its content of **1**.

In summary we revealed the uncommon emission behaviours of a silole (**1**) in this study. It has been a common 'law' that aggregation quenches light emission. What we observed here is exactly the opposite: light emission is induced by aggregation. The aggregation increased the emission efficiency of **1** by as high as two orders of magnitude (333 times). This is exceptionally rare, if not unprecedented, for small organic molecules.<sup>8</sup> Aggregation quenching has been the thorniest problem in the development of organic light-emitting diodes with high efficiencies. Our finding of aggregation-induced emission may stimulate new molecular engineering endeavours in the design of luminescent organics and polymers with highly emissive aggregation states.

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## Notes and references

<sup>†</sup> ITO = indium–tin oxide, CuPc = copper phthalocyanine, TPD = *N,N'*-diphenyl-*N,N'*-bis(3-methylphenyl)-1,1'-diphenyl-4,4'-diamine,  $\text{Alq}_3$  = tris(8-hydroxyquinolino)aluminum.

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